

Case/Application number: 10598826

Priority Filing Date:

Format for Search Results: No selection

Meaning of unusual acronyms or initialisms:

Identify the novelty:

Additional comments:

Please search the following attached claims (claims 1, 2, 11 and 12).

=> fil hcplus

FILE 'HCAPLUS' ENTERED AT 16:20:31 ON 15 AUG 2008

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FILE COVERS 1907 - 15 Aug 2008 VOL 149 ISS 8

FILE LAST UPDATED: 14 Aug 2008 (20080814/ED)

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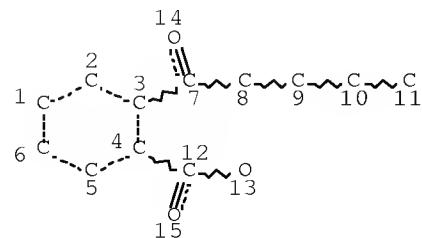
This file contains CAS Registry Numbers for easy and accurate substance identification.

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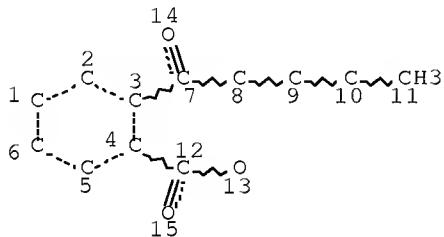
L23 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
 L25 128 SEA FILE=REGISTRY SSS FUL L23
 L26 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
 L27 38 SEA FILE=REGISTRY SUB=L25 SSS FUL L26
 L28 40 SEA FILE=HCAPLUS ABB=ON PLU=ON L27

=> d ibib abs hitstr 128 1-40

L28 ANSWER 1 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:1055762 HCAPLUS Full-text
 DOCUMENT NUMBER: 147:468949
 TITLE: Dipole-LUMO/Dipolarophile-HOMO Controlled Asymmetric Cycloadditions of Carbonyl Ylides Catalyzed by Chiral Lewis Acids
 AUTHOR(S): Suga, Hiroyuki; Ishimoto, Daisuke; Higuchi, Satoshi; Ohtsuka, Motoo; Arikawa, Tadashi; Tsuchida, Teruko; Kakehi, Akikazu; Baba, Toshihide
 CORPORATE SOURCE: Department of Chemistry and Material Engineering, Faculty of Engineering, Shinshu University, Wakasato, Nagano, 380-8553, Japan
 SOURCE: Organic Letters (2007), 9(21), 4359-4362
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 147:468949
 AB We have found the first successful example of reverse-electron-demand dipole-LUMO/dipolarophile-HOMO controlled cycloaddn. reactions between carbonyl

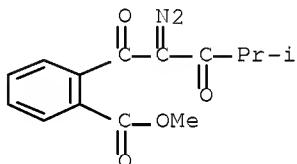
ylides, which were generated from o-methoxycarbonyl- α - diazoacetophenone and their acyl derivs. as precursors, and vinyl ether derivs. with high levels of asym. induction (97-77% ee) using chiral 2,6-(oxazolinyl)pyridine-Eu(III) or binaphthyldiimine-Ni(II) complexes as chiral Lewis acid catalysts.

IT 952687-64-8

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(dipole-LUMO/dipolarophile-HOMO controlled asym. cycloaddns. of carbonyl ylides catalyzed by chiral Lewis acids)

RN 952687-64-8 HCPLUS

CN Benzoic acid, 2-(2-diazo-4-methyl-1,3-dioxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 2 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:980459 HCPLUS [Full-text](#)

DOCUMENT NUMBER: 149:9951

TITLE: Design, synthesis and activity evaluation of novel selective serotonin reuptake inhibitors

AUTHOR(S): Yang, Jing; Wang, Xiao-Fang; Du, Guan-Hua; Qin, Fang; Wen, Hui; Yang, Guang-Zhong

CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, 100050, Peop. Rep. China

SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2007), 28(8), 1503-1507

CODEN: KTHPDM; ISSN: 0251-0790

PUBLISHER: Gaodeng Jiaoyu Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB During the past two decades, selective serotonin reuptake inhibitors (SSRIs) have been proved to be a safer and more effective resistance than the first-generation antidepressants (TCAs and MAOIs), and have gained incredible popularity. Based on the conformation anal. and pharmacophore information of SSRIs, flexible database searching from the NCI-3D and Maybridge-3D database was performed. Three classes of the new compds. structures were designed and 27 analogs were prepared and evaluated as potential antidepressant agents. Biphenylbenzamidine derivative showed good activity of affinity to the 5-HT transporter. It can be used as the leader structure for drug design with the objective of making more potent inhibitors against 5-HT transporter.

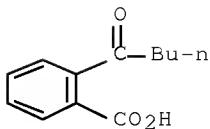
IT 550-37-8P 64624-87-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(design, synthesis and evaluation of selective serotonin reuptake inhibitors)

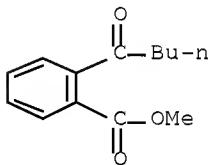
RN 550-37-8 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



RN 64624-87-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 3 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:833854 HCPLUS [Full-text](#)

DOCUMENT NUMBER: 148:315535

TITLE: High-performance liquid chromatography with atmospheric pressure chemical ionization and electrospray ionization mass spectrometry for analysis of Angelica sinensis

AUTHOR(S): Wang, Ya-Li; Liang, Yi-Zeng; Chen, Ben-Mei

CORPORATE SOURCE: Research Center of Modernization of Chinese Herbal Medicines, Central South University, Changsha, 410083, Peop. Rep. China

SOURCE: Phytochemical Analysis (2007), 18(4), 265-274

CODEN: PHANEL; ISSN: 0958-0344

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An HPLC-PAD-API/MS method for analyzing the chemical constituents of Angelica sinensis (*A. sinensis*) has been developed. ESI and APCI spectra, in both pos. ion and neg. ion modes, provided very useful information concerning the mol. wts. of detected compds. By comparing the retention times, UV spectra, mass spectra and mol. wts. of detected compds. with those published in literature, 15 constituents of *A. sinensis* could be tentatively identified. This technique involving combined MS information may provide an objective, reliable and rapid anal. method for the quality control and database research of traditional Chinese medicines.

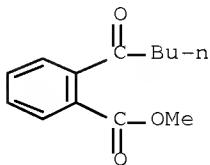
IT 64624-87-9

RL: ANT (Analyte); NPO (Natural product occurrence); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); USES (Uses)

(Angelica sinensis anal. by high-performance liquid chromatog. with atmospheric

pressure chemical ionization and electrospray ionization mass spectrometry)

RN 64624-87-9 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 4 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:809095 HCAPLUS Full-text

DOCUMENT NUMBER: 148:517475

TITLE: Stereoselective synthesis of 3-butylphthalide via CBS catalytic reduction

AUTHOR(S): Xu, Geng; Liu, Zhan Zhu; Yang, Jing Hua; Chen, Shi Zhi; Yang, Hui Ying

CORPORATE SOURCE: Institute of Materia Medica, Peking Union Medical College and Chinese Academy of Medical Science, Beijing, 100050, Peop. Rep. China

SOURCE: Chinese Chemical Letters (2007), 18(6), 653-655
 CODEN: CCLEE7; ISSN: 1001-8417

PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Optically active 3-butylphthalide of high enantiomeric excesses ($\leq 93\% \text{ ee}$) was synthesized by reduction of 2-pentanoylbenzoic ester with borane using B-methoxyoxazaborolidine as the chiral catalyst.

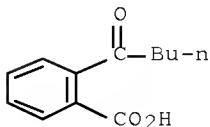
IT 550-37-8P, 2-Pentanoylbenzoic acid 1021950-15-1P, Benzyl 2-pentanoylbenzoate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

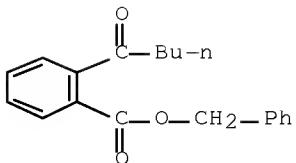
(asym. synthesis of butylphthalide via reduction with oxazaborolidine catalyst)

RN 550-37-8 HCAPLUS

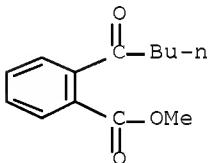
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



RN 1021950-15-1 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, phenylmethyl ester (CA INDEX NAME)



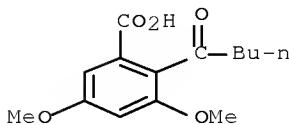
IT 64624-87-9P, Methyl 2-pentanoylbenzoate
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (asym. synthesis of butylphthalide via reduction with oxazaborolidine catalyst)
 RN 64624-87-9 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 5 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:602595 HCAPLUS Full-text
 DOCUMENT NUMBER: 147:180528
 TITLE: Rational design of inhibitors of VirA-VirG two-component signal transduction
 AUTHOR(S): Maresh, Justin; Zhang, Jin; Tzeng, Yih-Ling; Goodman, Nora A.; Lynn, David G.
 CORPORATE SOURCE: Department of Chemistry, Center for Fundamental and Applied Molecular Evolution, Emory University, Atlanta, GA, 30322, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(12), 3281-3286
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB VirA-VirG two-component system regulates the vir (virulence) operon in response to specific host factors (xenognosins) in the plant pathogen Agrobacterium tumefaciens. Using whole cell assays, stable inhibitors inspired by the labile natural benzoxazinone inhibitor HDMBOA are developed. It is found that aromatic aldehydes represent a minimal structural unit for activity. In particular, 3-hydroxy-4,6-dimethoxy-3H- isobenzofuran-1-one (HDI) was found to have the highest activity, making it the most potent developed inhibitor of virulence gene expression in Agrobacterium.
 IT 944558-07-0
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
 (rational design of inhibitors of VirA-VirG two-component signal

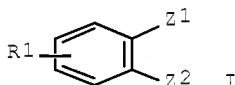
transduction based on maize root HDMBOA)
RN 944558-07-0 HCPLUS
CN Benzoic acid, 3,5-dimethoxy-2-(1-oxopentyl)- (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 6 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1261607 HCPLUS Full-text
DOCUMENT NUMBER: 144:6574
TITLE: Preparation of o-acylbenzoic acid derivatives from phthalic acid diesters
INVENTOR(S): Nishizawa, Yoshinori; Ichinose, Susumu
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005330218	A	20051202	JP 2004-149474	20040519
PRIORITY APPLN. INFO.:			JP 2004-149474	20040519
OTHER SOURCE(S):	CASREACT 144:6574; MARPAT 144:6574			
GI				

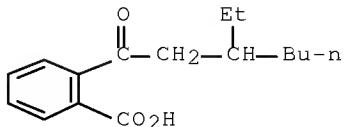


AB The derivs. I [R1 = H, halo, lower alkyl, lower alkoxy; Z1 = COR2 (R2 = alkyl); Z2 = CO2H], useful as intermediates for bioactive 3-substituted phthalides, are prepared by reacting R2MgX (R2 = same as above) with an excess amount of I [R1 = same as above; Z1, Z2 = CO2L (L = lower alkyl)] and hydrolyzing the resulting products. Thus, a THF/toluene solution of Me(CH2)7MgBr was added dropwise to a THF/toluene solution of 388.4 g o-C6H4(CO2Me)2 at 5° to give 134.6 g o-Me(CH2)7COC6H4CO2H.

IT 106462-12-8P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of o-acylbenzoic acids from phthalic acid diesters and Grignard reagents)

RN 106462-12-8 HCPLUS

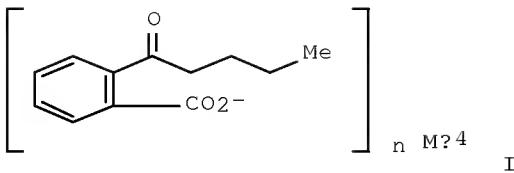
CN Benzoic acid, 2-(3-ethyl-1-oxoheptyl)- (CA INDEX NAME)



L28 ANSWER 7 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:1026918 HCPLUS Full-text
 DOCUMENT NUMBER: 143:299115
 TITLE: Novel 2-(α -n-pentanonyl)benzoates, their preparation and use
 INVENTOR(S): Liu, Quanzhi; Yang, Wenbin; Qin, Hua; Zhao, Xingkai;
 Ma, Xisheng
 PATENT ASSIGNEE(S): Team Academy of Pharmaceutical Science, Peop. Rep. China
 SOURCE: PCT Int. Appl., 35 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005087701	A1	20050922	WO 2004-CN602	20040604
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1560018	A	20050105	CN 2004-10007520	20040312
EP 1734031	A1	20061220	EP 2004-738206	20040604
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2007528878	T	20071018	JP 2007-502170	20040604
US 20070203233	A1	20070830	US 2006-598826	20060912
KR 809778	B1	20080304	KR 2006-720046	20060927
PRIORITY APPLN. INFO.:			CN 2004-10007520	A 20040312
			WO 2004-CN602	W 20040604

GI



AB The present invention relates to novel compds. 2-(α -n-pentanonyl)benzoates I (where n = 1, 2; M = Na⁺, Ca⁺, K⁺, Li⁺, iso-Pr amine, N,N'-Dibenzyl ethylenediamine, Benzyl amine, (S)- α -Me benzyl amine), their preparation method, the pharmaceutical composition containing the same, and their use in preparing the medicine for preventing and/or treating cardioischemia/cerbroischemia, thrombus and disorder of cardiac/cerebral circulation.

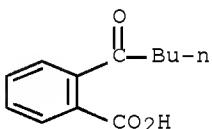
IT 864856-61-1P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(novel 2-(α -n-pentanonyl)benzoates, their preparation and use)

RN 864856-61-1 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, sodium salt (1:1) (CA INDEX NAME)



Na

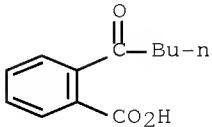
IT 864856-62-2P 864856-63-3P 864856-64-4P
864856-65-5P 864856-66-6P 864856-67-7P
864856-68-8P 864856-69-9P 864856-70-2P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(novel 2-(α -n-pentanonyl)benzoates, their preparation and use)

RN 864856-62-2 HCAPLUS

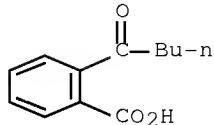
CN Benzoic acid, 2-(1-oxopentyl)-, potassium salt (1:1) (CA INDEX NAME)



K

RN 864856-63-3 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, calcium salt (2:1) (CA INDEX NAME)



●1/2 Ca

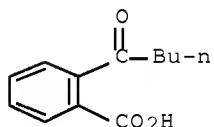
RN 864856-64-4 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, compd. with N,N'-bis(phenylmethyl)-1,2-ethanediamine (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 550-37-8

CMF C12 H14 O3



CM 2

CRN 140-28-3

CMF C16 H20 N2



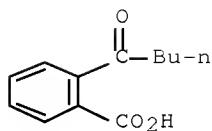
RN 864856-65-5 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, compd. with 2-methyl-2-propanamine (1:1) (CA INDEX NAME)

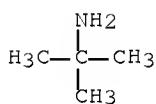
CM 1

CRN 550-37-8

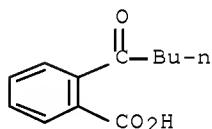
CMF C12 H14 O3



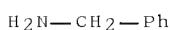
CM 2

CRN 75-64-9
CMF C4 H11 NRN 864856-66-6 HCPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, compd. with benzenemethanamine (1:1) (CA INDEX NAME)

CM 1

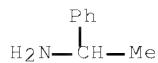
CRN 550-37-8
CMF C12 H14 O3

CM 2

CRN 100-46-9
CMF C7 H9 NRN 864856-67-7 HCPLUS
CN Benzoic acid, 2-(1-oxopentyl)-, compd. with α -methylbenzenemethanamine (1:1) (CA INDEX NAME)

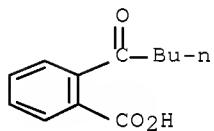
CM 1

CRN 618-36-0
 CMF C8 H11 N

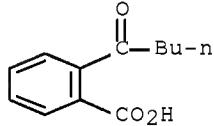


CM 2

CRN 550-37-8
 CMF C12 H14 O3

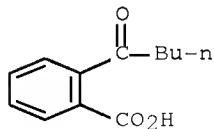


RN 864856-68-8 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, zinc salt (2:1) (CA INDEX NAME)



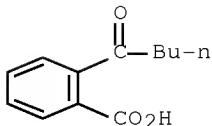
●1/2 Zn

RN 864856-69-9 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, magnesium salt (2:1) (CA INDEX NAME)



●1/2 Mg

RN 864856-70-2 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, lithium salt (1:1) (CA INDEX NAME)



● Li

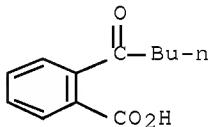
IT 550-37-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(novel 2-(α -n-pentanonyl)benzoates, their preparation and use)

RN 550-37-8 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 8 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:1000504 HCPLUS Full-text

DOCUMENT NUMBER: 141:242819

TITLE: Product class 4: organometallic complexes of copper

AUTHOR(S): Heaney, H.; Christie, S.

CORPORATE SOURCE: Dept. of Chemistry, University of Loughborough, Loughborough, LE11 3TU, UK

SOURCE: Science of Synthesis (2004), 3, 305-662
CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. The use of copper and related complexes in applications to organic synthesis is reviewed.

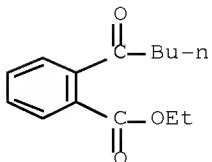
IT 131379-20-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(applications of copper and organocopper complexes to organic synthesis)

RN 131379-20-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, ethyl ester (CA INDEX NAME)

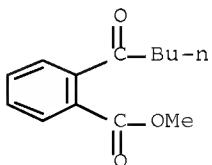


REFERENCE COUNT: 1706 THERE ARE 1706 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 9 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:129893 HCPLUS Full-text
 DOCUMENT NUMBER: 139:68703
 TITLE: Ruthenium(II)-catalyzed asymmetric transfer hydrogenation of carbonyl compounds with 2-propanol and ephedrine-type ligands
 AUTHOR(S): Everaere, Kathelyne; Mortreux, Andre; Carpentier, Jean-Francois
 CORPORATE SOURCE: Laboratoire de Catalyse de Lille, UPRESA 8010 CNRS, Villeneuve d'Ascq, 59652, Fr.
 SOURCE: Advanced Synthesis & Catalysis (2003), 345(1+2), 67-77
 CODEN: ASCAF7; ISSN: 1615-4150
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:68703

AB The development and application of Noyori's type catalysts based on ruthenium-arene complexes and simple chiral β -amino alcs. derived from ephedrine for the asym. transfer hydrogenation of 2-propanol to carbonyl substrates are studied. The influence of key parameters of the catalyst system has been studied systematically, resulting in particular in the design of the novel ligand (4-biphenylmethyl)norephedrine. The catalytic precursors and true active species could be isolated for the first time, enabling a complete structural description of the catalytic cycle and of probable deactivation pathways. Highly effective applications of those catalysts systems, i.e., the asym. redns. of simple aryl ketones and aryl β -keto esters, the synthesis of chiral phthalides and syn- β,δ -dihydroxy esters, are described.

IT 64624-87-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. transfer hydrogenation of carbonyl compds. with propanol in presence of ruthenium(II) complex catalysts and ephedrine-type ligands)
 RN 64624-87-9 HCPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 10 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:155152 HCPLUS Full-text
 DOCUMENT NUMBER: 135:5495
 TITLE: Stereoselective synthesis of 3-substituted phthalides

via asymmetric transfer-hydrogenation using well-defined ruthenium catalysts under neutral conditions
 AUTHOR(S): Everaere, K.; Scheffler, J.-L.; Mortreux, A.; Carpentier, J.-F.
 CORPORATE SOURCE: Groupe de Chimie Organique Appliquee, Laboratoire de Catalyse de Lille Associe au CNRS, Ecole Nationale Superieure de Chimie de Lille, Villeneuve d'Ascq, Fr.
 SOURCE: Tetrahedron Letters (2001), 42(10), 1899-1901
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:5495

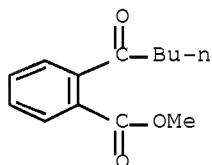
AB The asym. transfer-hydrogenation of Me 2-acylbenzoates and iso-Pr 3-acetylpyridine-2-carboxylate in 2-propanol, in the absence of base, with preformed Ru diamido or alkoxy-amido complex catalysts provides 3-alkylphthalides in high yields and 92-97% ee. The procedure is, however, not as efficient for the preparation of optically active 3-phenylphthalide.

IT 64624-87-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of phthalides via asym. transfer-hydrogenation with ruthenium catalysts under neutral conditions)

RN 64624-87-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 11 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1999:655809 HCPLUS Full-text
 DOCUMENT NUMBER: 131:272001
 TITLE: Method of storing active zero valent zinc metal and applications in organic synthesis
 INVENTOR(S): Rieke, Reuben D.
 PATENT ASSIGNEE(S): Board of Regents of the University of Nebraska, USA
 SOURCE: U.S., 33 pp., Cont.-in-part of U.S. Ser. No. 917,587, abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5964919	A	19991012	US 1995-432828	19950502
US 5358546	A	19941025	US 1992-830629	19920204

US 5756653	A	19980526	US 1995-432995	19950502
PRIORITY APPLN. INFO.:			US 1992-830629	A2 19920204
			US 1992-917587	B2 19920721

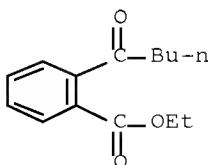
AB There is claimed a method of storing an active zerovalent Zn metal consisting of: (a) suspending in a container the active Zn in an ethereal, hydrocarbon, aromatic hydrocarbon or aprotic polar solvent at a temperature of between -20° to 30° under an inert atmospheric; and (b) sealing the container; wherein the active Zn is stored for six months without substantial loss of activity. An object of the invention (not claimed) is to produce a Zn species that is more reactive than those obtained from traditional methods. The zerovalent Zn species is directly produced by reaction of a reducing agent on a Zn salt, preferably Zn(CN)2. Another object of the invention (not claimed) is to produce a Zn species that is highly reactive towards oxidative addition. The organozinc reagent results from the reaction of the zerovalent Zn species and an organic compound having one or more stable anionic leaving groups. Yet another object of the invention (not claimed) is the direct production of a wide variety of organozinc compds., e.g., aryl, heterocyclic, arylalkyl, and polymeric Zn reagents that can undergo a number of valuable synthetic reactions. Still another object of the invention (not claimed) is to produce a wide variety of organozinc reagents that contain a broad spectrum of functional groups such as esters, ketones, nitrites, halides, amides, carbamates, epoxides, aldehydes, α,β-unsatd. enones (e.g., esters and ketones), sulfoxides, sulfones, etc. Furthermore, an object of the invention (not claimed) is the synthesis of new organic compds. or the synthesis of known organic compds. using more effective and/or more direct synthetic methods. Many examples of copper-mediated reactions of organozinc halides with acid chlorides, α,β-unsatd. ketones, allylic halides, YCH2C.tplbond.CCH2Y (Y = Cl, OTs), and H2C:CBrCH2Br and palladium-catalyzed reactions with acid chlorides and aryl and vinyl halides are given. Also, the use of highly reactive Zn in the preparation of polythiophenes and poly-para-phenylene is illustrated; the 1st reported 3-alkylpolythiophene that is >99% regioregular is included. The examples are the same as in an earlier patent (WO 93/15086; Chemical Abstrs. accession number 120:54698).

IT 131379-20-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(method of storing active zero valent zinc metal and applications in
organic synthesis)

RN 131379-20-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 12 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:343348 HCPLUS Full-text

DOCUMENT NUMBER: 129:113627

ORIGINAL REFERENCE NO.: 129:23223a, 23226a

TITLE: Liquid chromatographic-electrospray mass spectrometric study of the phthalides of Angelica sinensis and chemical changes of Z-ligustilide

AUTHOR(S): Lin, Long-Ze; He, Xian-Guo; Lian, Li-Zhi; King, Wayne; Elliott, Jerry

CORPORATE SOURCE: Research Laboratory of Natural Products Chemistry, East Earth Herb Inc., 4091 W. 11th Avenue, Eugene, OR, 97402, USA

SOURCE: Journal of Chromatography, A (1998), 810(1 + 2), 71-79
 CODEN: JCRAEY; ISSN: 0021-9673

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

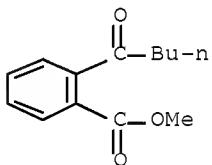
LANGUAGE: English

AB High-performance liquid chromatog.-electrospray ionization-mass spectrometry has been applied to analyze the chemical constituents of Danggui (the rhizome of Angelica sinensis) and to study chemical changes of Z-ligustilide. Twelve phthalides were unambiguously identified as senkyunolide I (3), senkyunolide H (4), sedanenolide (8), butylphthalide (9), E-ligustilide (13), Z-ligustilide (14), Z-butylidenephthalide (15), Z,Z'-6.8',7.3'- diligustilide (16), angelicide (17), levistolide A (18), Z-ligustilide dimer E-232 (19) and Z,Z'-3.3',8.8'-diligustilide (20) in Danggui extract. The existence of 12 other phthalides (2, 5-7, 11, 12, 22-27), ferulic acid (1) and coniferyl ferulate (10) in Danggui extract has also been demonstrated. Phthalides 3, 4, 16-18 and 20 were determined to be the products from chemical change of Z-ligustilide. This is the first report of the existence of 16 compds. (2-8, 10-12, 20, 22-25 and 27) in Danggui extract

IT 64624-87-9
 RL: ANT (Analyte); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
 (liquid chromatog.-electrospray mass spectrometric study of the phthalides of Angelica sinensis and chemical changes of Z-ligustilide)

RN 64624-87-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 13 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1998:198830 HCPLUS Full-text
 DOCUMENT NUMBER: 128:316878
 ORIGINAL REFERENCE NO.: 128:62621a,62624a
 TITLE: Study on the metabolites of dl-3-n-butylphthalide in rats
 AUTHOR(S): Wang, Chunhua; Feng, Yipu; Wu, Yuanliu
 CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Science and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
 SOURCE: Yaoxue Xuebao (1997), 32(9), 641-646

CODEN: YHHPAL; ISSN: 0513-4870

PUBLISHER: Chinese Academy of Medical Sciences, Institute of
Materia Media

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The metabolites of dl-3-n-butylphthalide (NBP) were studied in rats. Two main in vitro metabolites of NBP, M I and M II, were isolated and purified from rat liver microsome incubating system by using HPLC. Their structure was determined by spectral studies (UV, ^1H - NMR, MS). Within 24 h following ig 3H-NBP, the total radioactivity excreted in urine and feces was 73.7% of the dose. Comparing with previous study, within 72 h following ig NBP, the total prototype drug excreted in urine and feces was 2.53% of the dose. This result excludes the possibility that NBP accumulates in vivo. The urine and brain homogenate of the rats (ig 3H-NBP) were analyzed by TLC. M I and M II were found in urine and M I was found in brain only. The ratio of radioactive M I to drug was 1 : 1 in rat brain within 1 h following ig 3H-NBP. The results suggest that M I might be an active metabolite.

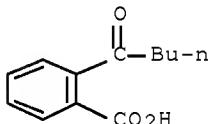
IT 550-37-8

RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)

(study on the metabolites of dl-3-n-butylphthalide in rats)

RN 550-37-8 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 14 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:804990 HCPLUS Full-text

DOCUMENT NUMBER: 128:75228

ORIGINAL REFERENCE NO.: 128:14715a, 14718a

TITLE: Microbial asymmetric syntheses of 3-alkylphthalide derivatives

AUTHOR(S): Kitayama, Takashi

CORPORATE SOURCE: Department of Agricultural Chemistry, Faculty of Agriculture, Kinki University, Nara, 631, Japan

SOURCE: Tetrahedron: Asymmetry (1997), 8(22), 3765-3774

CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:75228

AB Phthalide derivs., almost all of which have an S-configuration, have a wide range of activity and exist in *Angerica sinensis* Diels and *Sligusticum wallichii* Franch. For the first time, optically active (S)-3-methylphthalide derivs. were synthesized using two methods, asym. microbial reduction and microbial hydroxylation. For the first method, Me 2-acetylbenzoate was synthesized as a substrate, which was reduced asym. by *Geotrichum candidum* IFO 34614 to obtain (S)-3-methylphthalide in 92% yield (99% enantiomeric excess, ee). For the second method, 2-ethylbenzoic acid was employed as a substrate

which was hydroxylated asym. at the benzylic position by either Pseudomonas putida ATCC 12633 or Aspergillus niger IFO 6661, whose fermentation was induced by o-toluic acid, to obtain (S)-3-methylphthalide in 80% yield (99% ee). (S)-3-Butylphthalide and (S)-3-octylphthalide were obtained in the same manner in 12% yield (ee=99%) and 10% yield (ee=99%), resp.

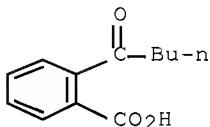
IT 550-37-8P, 2-Pentanoylbenzoic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(microbial asym. syntheses of 3-alkylphthalide derivs.)

RN 550-37-8 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



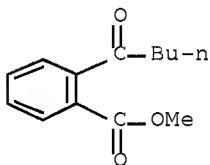
IT 64624-87-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(microbial asym. syntheses of 3-alkylphthalide derivs.)

RN 64624-87-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



REFERENCE COUNT:

24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 15 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:766493 HCPLUS [Full-text](#)

DOCUMENT NUMBER: 128:3590

ORIGINAL REFERENCE NO.: 128:779a, 782a

TITLE: Synthesis of (Z)-3-butylidene-4,5-dihydroxyphthalide

AUTHOR(S): Li, Shaobai; Yan, Fulin; Wang, Zhiwei; Li, Yulin

CORPORATE SOURCE: State Key Laboratory of Applied Organic Chemistry, Institute of Organic Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China

SOURCE: Huaxue Yanjiu Yu Yingyong (1997), 9(4), 338-342

CODEN: HYYIFM; ISSN: 1004-1656

PUBLISHER: Huaxue Yanjiu Yu Yingyong Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB (Z)-3-Butylideneephthalide (I) and its derivs. were isolated as the Umbelliferae which are used frequently as an ingredient in the prescriptions of traditional Chinese medicine. (Z)-3-butylidene-4,5- dihydroxyphthalide

(II), an inhibitor of prostaglandin F_{2α}, is a similar to I. II was prepared starting from 3,4-dimethoxybenzyl alc. or 3,4-methyldenedioxybenzyl alc. employing heteroatom directed lithiation reaction on aromatic compound

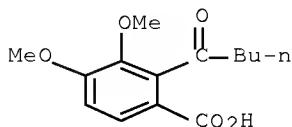
IT 198754-73-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of (Z)-3-butylidene-4,5-dihydroxyphthalide)

RN 198754-73-3 HCAPLUS

CN Benzoic acid, 3,4-dimethoxy-2-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 16 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:423919 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 125:137014

ORIGINAL REFERENCE NO.: 125:25537a,25540a

TITLE: Depsidone chemical transformations in an extract of the lichen *Stereocaulon azoreum*

AUTHOR(S): Gonzalez, Antonio G.; Rodriguez, Elsa M.; Bermejo, Jaime

CORPORATE SOURCE: Centro Productos Naturales Organicos, La Laguna, 38206, Spain

SOURCE: Anales de Quimica (1995), 91(5-6), 461-466

CODEN: ANQUEX; ISSN: 1130-2283

PUBLISHER: Real Sociedad Espanola de Quimica

DOCUMENT TYPE: Journal

LANGUAGE: English

AB If the crude residue of an acetone extract of *Stereocaulon azoreum* was redissolved in a hexane:chloroform:methanol mixture and kept in the dark for three months, chemical transformations of stictic, cryptostictic and lobaric acids took place. The structures of the transformation products were established by mass spectrometry and ¹H-¹³C-NMR spectral anal.

IT 179691-10-2 179691-11-3 179691-12-4

179691-13-5 179691-14-6

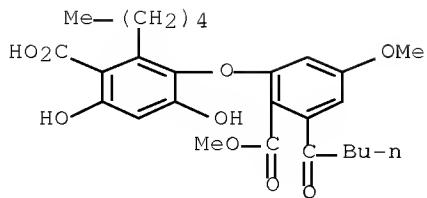
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); FMU (Formation, unclassified); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)

(depsidone chemical transformations in an extract of the lichen

Stereocaulon
azoreum)

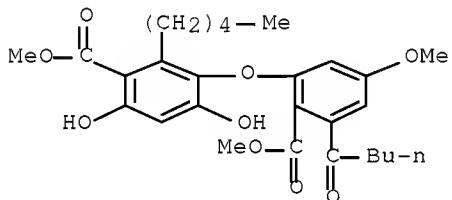
RN 179691-10-2 HCAPLUS

CN Benzoic acid, 4,6-dihydroxy-3-[5-methoxy-2-(methoxycarbonyl)-3-(1-oxopentyl)phenoxy]-2-pentyl- (CA INDEX NAME)



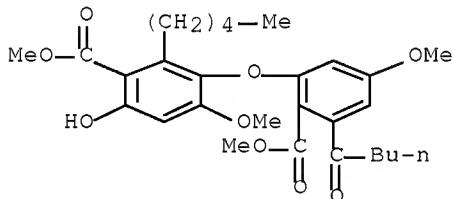
RN 179691-11-3 HCPLUS

CN Benzoic acid, 4,6-dihydroxy-3-[5-methoxy-2-(methoxycarbonyl)-3-(1-oxopentyl)phenoxy]-2-pentyl-, methyl ester (CA INDEX NAME)



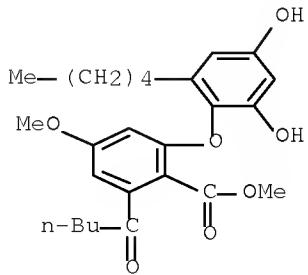
RN 179691-12-4 HCPLUS

CN Benzoic acid, 6-hydroxy-4-methoxy-3-[5-methoxy-2-(methoxycarbonyl)-3-(1-oxopentyl)phenoxy]-2-pentyl-, methyl ester (CA INDEX NAME)



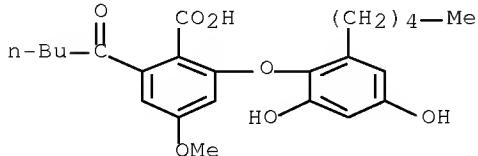
RN 179691-13-5 HCPLUS

CN Benzoic acid, 2-(2,4-dihydroxy-6-pentylphenoxy)-4-methoxy-6-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



RN 179691-14-6 HCAPLUS

CN Benzoic acid, 2-(2,4-dihydroxy-6-pentylphenoxy)-4-methoxy-6-(1-oxopentyl)-(CA INDEX NAME)



L28 ANSWER 17 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:198474 HCAPLUS Full-text

DOCUMENT NUMBER: 124:343016

ORIGINAL REFERENCE NO.: 124:63707a,63710a

TITLE: Efficient general asymmetric syntheses of
3-substituted 1(3H)-isobenzofuranones in very high
enantiomeric excessAUTHOR(S): Ramachandran, P. Veeraraghavan; Chen, Guang-Ming;
Brown, Herbert C.CORPORATE SOURCE: H.C. Brown and R. B. Wetherill Lab. Chem., Purdue
Univ., West Lafayette, IN, 47907-1393, USASOURCE: Tetrahedron Letters (1996), 37(13), 2205-8
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:343016

AB The intermol. asym. reduction of Me o-(1-oxoalkyl)benzoates with β -chlorodiisopinocampheylborane provides, after workup, 3-alkylphthalides in $\geq 97\%$ ee. Unfortunately, this procedure is not as efficient for the preparation of 3-arylphthalides. However, an intramol. reduction of B-(o-benzoylbenzoyloxy)diisopinocampheylborane, readily prepared by the treatment of o-benzyl benzoic acid with diisopinocampheylborane, provides 3-phenylphthalide in $\geq 96\%$ ee.

IT 550-37-8, Benzoic acid, 2-(1-oxopentyl)- 64624-87-9,

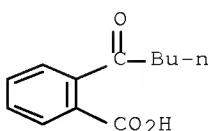
Benzoic acid, 2-(1-oxopentyl)-, methyl ester

RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. syntheses of 3-substituted 1(3H)-isobenzofuranones)

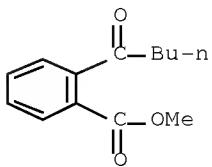
RN 550-37-8 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



RN 64624-87-9 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



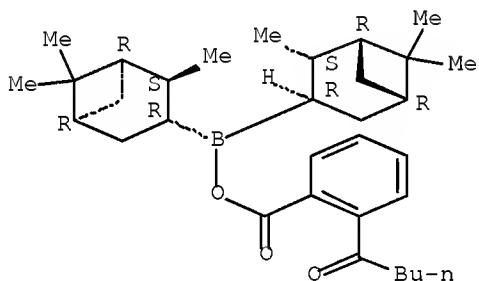
IT 176723-41-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. syntheses of 3-substituted 1(3H)-isobenzofuranones)

RN 176723-41-4 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, anhydride with bis(2,6,6-trimethylbicyclo[3.1.1]hept-3-yl)borinic acid, [1R-[1 α ,2 β ,3 α (1R*,2S*,3R*,5R*),5 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 18 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:837200 HCAPLUS Full-text

DOCUMENT NUMBER: 123:313625

ORIGINAL REFERENCE NO.: 123:56215a,56218a

TITLE: Syntheses of ligustilide and (\pm)-sedanenolide

AUTHOR(S): Li, Shao-Bai; Zhang, Shao-Ming; Li, Yu-Lin

CORPORATE SOURCE: Inst. of Organic Chemistry, Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China

SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1995), 16(9), 1420-2

CODEN: KTHPDM; ISSN: 0251-0790

PUBLISHER: Gaodeng Jiaoyu Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

OTHER SOURCE(S): CASREACT 123:313625

AB Z-ligustilide and sedanenolide are important naturally 3-alkylphthalide analogs occurring in many plants belonging to the Umbelliferae. They have antispasmodic antiasthmatic and smooth muscle relaxing activities. Herein the synthesis of (\pm)-sedanenolide is described, starting from phthalic anhydride as starting material. The key step in the synthesis is the Birch reduction of

3(Z)-butylenephthalide, 3-methoxy-3-butyphthalide and Me o-valerylbenzoate. The yield in this step is 44%-60%. The synthesis of ligustilide was studied.

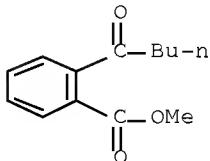
IT 64624-87-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(syntheses of ligustilide and (\pm)-sedanenolide via Birch reduction)

RN 64624-87-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 19 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:742952 HCPLUS Full-text

DOCUMENT NUMBER: 123:143629

ORIGINAL REFERENCE NO.: 123:25577a,25580a

TITLE: Preparation of 4,5-dihydro-3-(hydroxy)alkyl phthalides

INVENTOR(S): Li, Shaobai; Zhang, Shaoming; Li, Yulin

PATENT ASSIGNEE(S): Lanzhou University, Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 5 pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1087633	A	19940608	CN 1992-111279	19920930
CN 1034808	C	19970507		

PRIORITY APPLN. INFO.: CN 1992-111279 19920930

AB Title compds. were prepared by Birch reduction of o-acylbenzoates or 3-alkyl(idene)phthalides optionally substituted with a hydroxyl or carbonyl group on the alkyl(idene) group in liquid ammonia or amine by Na, Li, or K.

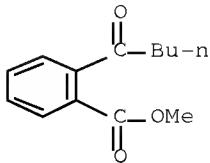
IT 64624-87-9, Methyl 2-valerylbenzoate

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 4,5-dihydro-3-(hydroxy)alkyl phthalides)

RN 64624-87-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 20 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1994:54698 HCPLUS Full-text
 DOCUMENT NUMBER: 120:54698
 ORIGINAL REFERENCE NO.: 120:9991a, 9994a
 TITLE: Preparation of highly reactive forms of zinc and reagents therefrom
 INVENTOR(S): Rieke, Rueben D.
 PATENT ASSIGNEE(S): University of Nebraska, USA
 SOURCE: PCT Int. Appl., 122 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9315086	A1	19930805	WO 1992-US8542	19921007
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
US 5358546	A	19941025	US 1992-830629	19920204
AU 9227878	A	19930901	AU 1992-27878	19921007
US 5756653	A	19980526	US 1995-432995	19950502
PRIORITY APPLN. INFO.:			US 1992-830629	A 19920204
			US 1992-917587	A 19920721
			WO 1992-US8542	A 19921007

OTHER SOURCE(S): CASREACT 120:54698

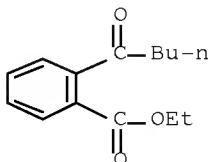
AB The preparation of novel zerovalent zinc species and organozinc reagents are described. The zerovalent zinc species is directly produced by action of a reducing agent on a zinc salt, preferably Zn(CN)2. The organozinc reagent is prepared by reaction of the zerovalent zinc species and an organic compound having one or more stable anionic leaving groups. These organozinc reagents include a wide spectrum of functional groups in the organic radical, and are useful in a variety of reaction schemes. Thus, reaction of Zn(CN)2 with lithium in the presence of naphthalene in THF gave highly reactive Zn metal which on treatment with 4-BrC6H4Me gave 100% 4-MeC6H4ZnBr (I). The reaction of I with various organic halides are described.

IT 131379-20-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

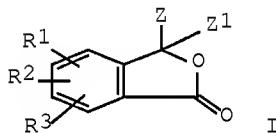
RN 131379-20-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, ethyl ester (CA INDEX NAME)

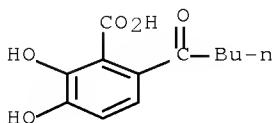


L28 ANSWER 21 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1992:469721 HCPLUS Full-text
 DOCUMENT NUMBER: 117:69721
 ORIGINAL REFERENCE NO.: 117:12259a,12262a
 TITLE: Preparation of phthalide derivatives as prostaglandin F_{2α} inhibitors
 INVENTOR(S): Ogawa, Yoshimitsu; Hosaka, Kunio; Kubota, Kiyoshi;
 Chin, Masao
 PATENT ASSIGNEE(S): Tsumura K. K., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

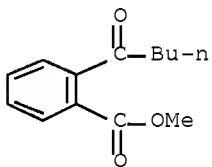
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04077480	A	19920311	JP 1990-189436	19900719
PRIORITY APPLN. INFO.:			JP 1990-189436	19900719
OTHER SOURCE(S):	MARPAT	117:69721		
GI				



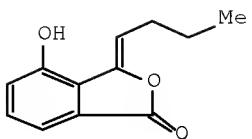
AB The title compds. (I; Z = Bu; Z1 = H, OH; or Z,Z1 = CHPr; R1-R3 = MeO, OH, H) are prepared. Thus, metalation of 6,7-dimethoxyphthalide (preparation given) with 1.6 M BuLi in (Me₂CH)₂NH/THF followed by a solution of ZnCl₂ in THF AT -40° and reaction with a solution of n-butyraldehyde at -40° gave 77.8 % 3-(1-hydroxybutyl)-6,7-dimethoxyphthalide. Mesylation of this with MeSO₂Cl in pyridine/benzene under reflux and treatment of the resulting 3-(1-mesyloxybutyl)-6,7-dimethoxyphthalide with DBU in refluxing benzene gave 22 % (Z)- and (E)-3-butylidene-6,7-dimethoxyphthalide. (Z)-3-Butylidene-5,6-dihydroxyphthalide at 5 × 10⁻⁶ g/mL in vitro inhibited 50.7 ± 7.3% prostaglandin F_{2α}. A total of 27 I were prepared
 IT 138350-82-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as prostaglandin F_{2α} inhibitor)
 RN 138350-82-0 HCPLUS
 CN Benzoic acid, 2,3-dihydroxy-6-(1-oxopentyl)- (CA INDEX NAME)



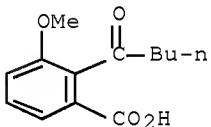
L28 ANSWER 22 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1992:444606 HCAPLUS Full-text
 DOCUMENT NUMBER: 117:44606
 ORIGINAL REFERENCE NO.: 117:7855a, 7858a
 TITLE: A phthalide and 2-farnesyl-6-methyl benzoquinone from Ligusticum chuanxiong
 AUTHOR(S): Naito, Takashi; Niitsu, Kazuaki; Ikeya, Yukinobu;
 Okada, Minoru; Mitsuhashi, Hiroshi
 CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ibaraki,
 300-11, Japan
 SOURCE: Phytochemistry (1992), 31(5), 1787-9
 CODEN: PYTCAS; ISSN: 0031-9422
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A new phthalide, senkyunolide Q, and 2-farnesyl-6-Me benzoquinone, senkyunone, along with senkyunolide M, 2-methoxy-4-(3-methoxy-1-propenyl)- phenol, and 2-(1-oxo-pentyl)-benzoic acid Me ester were isolated from the rhizome of Ligusticum chuanxiong. On the basis of spectral analyses and chemical methods, the structures of senkyunolide Q and senkyunone were proven to be (6RS,7SR)-3-butyldene-4,5,6,7-tetrahydro-7-hydroxy-6-(1-oxobutyl)- phthalide and (2'E,6'E)-2-farnesyl-6-methyl-p-benzoquinone, resp.
 IT 64624-87-9
 RL: BIOL (Biological study)
 (from Ligusticum chuanxiong)
 RN 64624-87-9 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



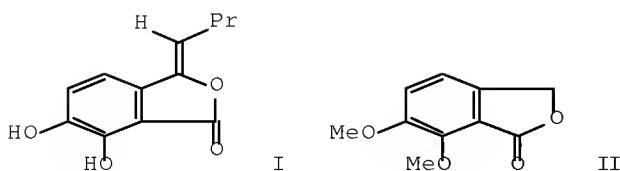
L28 ANSWER 23 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1992:128551 HCAPLUS Full-text
 DOCUMENT NUMBER: 116:128551
 ORIGINAL REFERENCE NO.: 116:21755a, 21758a
 TITLE: Synthesis of (Z)-3-butyldene-4-hydroxyphthalide
 AUTHOR(S): Ogawa, Y.; Hosaka, K.; Chin, M.; Mitsuhashi, H.
 CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ami, 300-11, Japan
 SOURCE: Synthetic Communications (1992), 22(2), 315-21
 CODEN: SYNAV; ISSN: 0039-7911
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 116:128551
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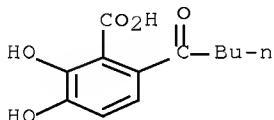
AB (Z)-3-Butylidene-4-hydroxyphthalide (I) was synthesized regio- and stereoselectively from 3-methoxybenzyl alc. in 4 steps involving regioselective lithiation and alkylation with BuCHO, oxidation with Bu4N+MnO4-, intramol. cyclization in presence of SOC12, and O-demethylation.
IT 116541-39-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclization of, in presence of thionyl chloride)
RN 116541-39-0 HCPLUS
CN Benzoic acid, 3-methoxy-2-(1-oxopentyl)- (CA INDEX NAME)



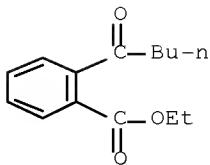
L28 ANSWER 24 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:41224 HCPLUS Full-text
DOCUMENT NUMBER: 116:41224
ORIGINAL REFERENCE NO.: 116:7065a, 7068a
TITLE: Synthesis of (Z)-3-butylidene-6,7-dihydroxyphthalide
AUTHOR(S): Ogawa, Yoshimitsu; Hosaka, Kunio; Chin, Masao;
Mitsuhashi, Hiroshi
CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ibaraki,
300-11, Japan
SOURCE: Heterocycles (1991), 32(9), 1737-44
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:41224
GI



AB The title compound I was first synthesized from dimethoxyphthalide II in 3 steps and its structure was synthetically confirmed.
 IT 138350-82-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of)
 RN 138350-82-0 HCPLUS
 CN Benzoic acid, 2,3-dihydroxy-6-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 25 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1991:81102 HCPLUS Full-text
 DOCUMENT NUMBER: 114:81102
 ORIGINAL REFERENCE NO.: 114:13829a,13832a
 TITLE: The direct formation of functionalized alkyl(aryl)zinc halides by oxidative addition of highly reactive zinc with organic halides and their reactions with acid chlorides, α,β -unsaturated ketones, and allylic, aryl, and vinyl halides
 AUTHOR(S): Zhu, Lishan; Wehmeyer, Richard M.; Rieke, Reuben D.
 CORPORATE SOURCE: Dep. Chem., Univ. Nebraska-Lincoln, Lincoln, NE,
 68588-0304, USA
 SOURCE: Journal of Organic Chemistry (1991), 56(4), 1445-53
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 114:81102
 AB Highly reactive zinc, prepared by reduction of ZnCl_2 with lithium naphthalenide, readily undergoes oxidative addition to alkyl, aryl, and vinyl halides under mild conditions to generate the corresponding organozinc compds. in excellent yields. Significantly, the reaction will tolerate a spectrum of functional groups on the organic halides. Accordingly, this approach can now be used to prepare a wide variety of highly functionalized organozinc compds. In the presence of $\text{Cu}(\text{I})$ salts, the organozinc compds. cross-couple with acid chlorides, conjugatively add to α,β -unsatd. ketones, and regioselectively undergo $\text{SN}2'$ substitution reactions with allylic halides. They also cross-couple with aryl or vinyl halides with $\text{Pd}(\text{0})$ catalysts.
 IT 131379-20-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 131379-20-9 HCPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, ethyl ester (CA INDEX NAME)



L28 ANSWER 26 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:98368 HCPLUS Full-text

DOCUMENT NUMBER: 112:98368

ORIGINAL REFERENCE NO.: 112:16727a,16730a

TITLE: Phthalides as prostaglandin F 2 α inhibitors and
their preparationINVENTOR(S): Ogawa, Yoshimitsu; Chin, Masao; Hosaka, Kunio; Kubota,
Kiyoshi

PATENT ASSIGNEE(S): Tsumura and Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

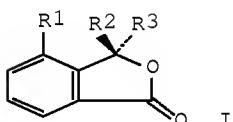
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 01199958	A	19890811	JP 1987-182228	19870723
PRIORITY APPLN. INFO.:			JP 1987-182228	19870723
OTHER SOURCE(S):	MARPAT	112:98368		
GI				



AB The title compds. I (R1 = H, MeO; when R2 is Bu, R3 is H, or when R2 is H, R3 = Bu; excluding the case where R1 = R2 = H and R3 = Bu), useful as prostaglandin F 2 α inhibitors, were prepared. A mixture of (-)-3-butyl-1-hydroxy-4-methoxy-2-oxindan, AgNO₃, and NaOH in MeOH-H₂O was stirred at room temperature for 1 h to give (-)-4-methoxy-3-butylphthalide (II). II in vitro inhibited prostaglandin F 2 α by 29.7%.

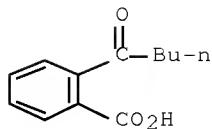
IT 550-37-8P 64624-87-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

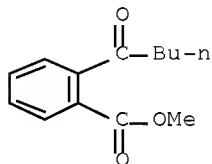
(preparation and reaction of, in preparation of prostaglandin F 2 α inhibitor)

RN 550-37-8 HCPLUS

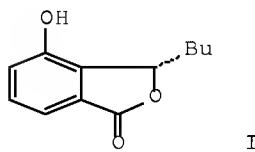
CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



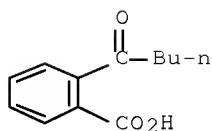
RN 64624-87-9 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



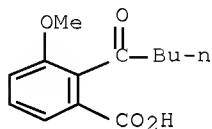
L28 ANSWER 27 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1990:76773 HCAPLUS Full-text
 DOCUMENT NUMBER: 112:76773
 ORIGINAL REFERENCE NO.: 112:13115a,13118a
 TITLE: Synthesis of (-)-3-butyl-4-hydroxyphthalide
 AUTHOR(S): Ogawa, Yoshimitsu; Hosaka, Kunio; Chin, Masao;
 Mitsuhashi, Hiroshi
 CORPORATE SOURCE: Res. Inst. Biol. Chem., Tsumura and Co., Ami, 300-11,
 Japan
 SOURCE: Heterocycles (1989), 29(5), 865-72
 CODEN: HTCYAM; ISSN: 0385-5414
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 112:76773
 GI



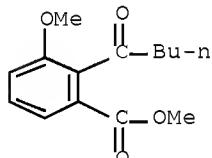
AB (-)-3-Butyl-4-hydroxyphthalide (I) was synthesized enantioselectively and its absolute stereochem. at C-3 was determined to be S.
 IT 550-37-8, 2-Valerylbenzoic acid 116541-39-6,
 3-Methoxy-2-valerylbenzoic acid
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (esterification of)
 RN 550-37-8 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



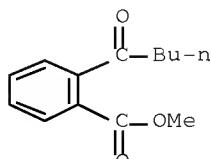
RN 116541-39-0 HCAPLUS
 CN Benzoic acid, 3-methoxy-2-(1-oxopentyl)- (CA INDEX NAME)



IT 124831-72-7P, Methyl 3-methoxy-2-valerylbenzoate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and attempted reduction of)
 RN 124831-72-7 HCAPLUS
 CN Benzoic acid, 3-methoxy-2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)

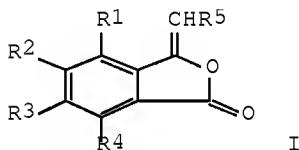


IT 64624-87-9P, Methyl 2-valerylbenzoate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reduction of)
 RN 64624-87-9 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



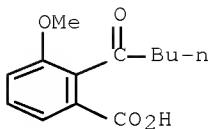
ACCESSION NUMBER: 1988:528817 HCPLUS Full-text
 DOCUMENT NUMBER: 109:128817
 ORIGINAL REFERENCE NO.: 109:21457a, 21460a
 TITLE: Preparation of phthalide derivatives as prostaglandin F_{2α} inhibitors
 INVENTOR(S): Ogawa, Yoshimitsu; Chin, Masao; Hosaka, Kunio; Kubota, Kiyoshi
 PATENT ASSIGNEE(S): Tsumura Juntendo, Inc., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63083081	A	19880413	JP 1986-228264	19860929
JP 07108906	B	19951122		
PRIORITY APPLN. INFO.:			JP 1986-228264	19860929
OTHER SOURCE(S):	MARPAT	109:128817		
GI				

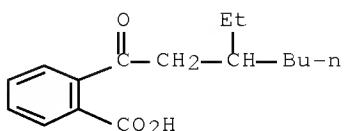


AB The title compds. [I; R₁ = H, OH, OMe, NO₂; R₂ = H, OH, OMe, OCH₂OMe; R₃ = H, OMe; R₄ = H, NO₂; R₅ = H, alkyl, (CH₂)₃CO₂H, (CH₂)₃CO₂Et, (CH₂)₄OH], useful as prostaglandin F_{2α} inhibitors, are prepared Cycloamidation of 3,4-(MeO)₂C₆H₃CO₂Cl with 2-amino-2-methyl-4-propanol and then treatment of the resultant amide with SOCl₂ gave 83% 2-(3,4-dimethoxyphenyl)-4,4-dimethyloxazoline which was reacted with BuLi and then paraformaldehyde at -45° to give 77% 4,5-dimethoxyphthalide (II). Reaction of II with n-PrCHO in the presence of n-BuLi, (Me₂CH)₂NH, and ZnCl₂ in THF at -40° overnight gave 97% 4,5-dimethoxy-3-(1-hydroxybutyl)-phthalide which in C₆H₆ was refluxed with MeClSO₂ in the presence of pyridine to give 99% 4,5-dimethoxy-3-(1-methanesulfonyloxybutyl)phthalide and the elimination reaction of the latter by refluxing in the presence of 1,8-diazabicyclo[5.4.0]undec-7-ene in C₆H₆ to give 74% (Z)- and 4.0% (E)-I (R₁ = R₂ = OMe, R₃ = R₄ = H, R₅ = Pr). Also, (Z)-I (R₁ = OH, R₂-R₄ = H, R₅ = Pr) at 5 × 10⁻⁸ g/mL in EtOH showed 48% inhibition of rat uterus contraction generated by prostaglandin F_{2α}.

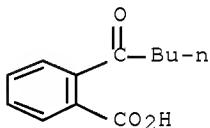
IT 116541-39-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclocondensation of)
 RN 116541-39-0 HCPLUS
 CN Benzoic acid, 3-methoxy-2-(1-oxopentyl)- (CA INDEX NAME)



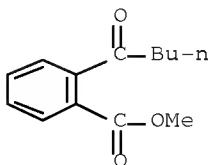
L28 ANSWER 29 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1987:62796 HCPLUS Full-text
 DOCUMENT NUMBER: 106:62796
 ORIGINAL REFERENCE NO.: 106:10271a
 TITLE: Mitogenicity of peroxisome proliferators in monolayers of adult rat hepatocytes
 AUTHOR(S): Bieri, F.; Bentley, P.; Waechter, F.; Staebli, W.
 CORPORATE SOURCE: Cent. Toxicol. Unit, Ciba-Geigy Ltd., Basel, 4002, Switz.
 SOURCE: Food and Chemical Toxicology (1986), 24(6-7), 709
 CODEN: FCTOD7; ISSN: 0278-6915
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The induction of peroxisomal enzymes and of replicative DNA synthesis were studied to examine the possible interrelation between these effects and to classify their importance in the carcinogenic process. The time course and reversibility of both effects were superimposable, but the dose response differed, being linear $\leq 100 \mu\text{g/mL}$ for peroxisomal enzyme induction, and showing a maximum at $10 \mu\text{g/mL}$ for induction of DNA synthesis. Several substances (e.g., prostaglandin synthesis inhibitors and antioxidants) were added to the culture medium to alter either replicative DNA synthesis or the oxidative effects resulting from peroxisome proliferation. The 2 parameters seemed to be altered independently, providing no evidence of any direct correlation. Dose-response curves with known peroxisome proliferators and related compds. indicated that the mitogenic potency of the proliferators could not be predicted from their effects on the peroxisomal compartment. Ranking of the substances according to their ability to induce replicative DNA synthesis in cultured hepatocytes was more in agreement with their hepatomegalic potency than was their ranking as peroxisome proliferators. The mitogenic potency of the substance and the peroxisome proliferation should be measured when the monolayers of adult rat hepatocytes are used to assess the possible hepatocarcinogenicity of the test substances.
 IT 106462-12-8
 RL: BIOL (Biological study)
 (peroxisome proliferator, mitogenicity of, in hepatocytes,
 hepatocarcinogenesis in relation to)
 RN 106462-12-8 HCPLUS
 CN Benzoic acid, 2-(3-ethyl-1-oxoheptyl)- (CA INDEX NAME)



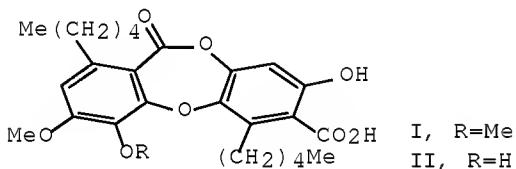
L28 ANSWER 30 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1981:602924 HCAPLUS Full-text
 DOCUMENT NUMBER: 95:202924
 ORIGINAL REFERENCE NO.: 95:33897a,33900a
 TITLE: Deactivation of triplet phenyl alkyl ketones by conjugatively electron-withdrawing substituents
 AUTHOR(S): Wagner, Peter J.; Siebert, Elizabeth J.
 CORPORATE SOURCE: Dep. Chem., Michigan State Univ., East Lansing, MI, 48824, USA
 SOURCE: Journal of the American Chemical Society (1981), 103(24), 7329-35
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Cyano, carbomethoxy and acyl para substituents decrease the triplet reactivity of PhCOBu (γ -H abstraction); comparable meta substituents increase reactivity. Spectroscopic results indicate that para (-R) substituents lower π,π^* triplet energies so much more than n,π^* energies that the lowest triplets become largely π,π^* in nature. Meta (-R) substituents do not stabilize π,π^* triplets enough to invert triplet levels. Both substitution patterns support a largely 1,4-biradical structure for the lowest π,π^* triplet of acylbenzenes. Ortho substituents show the usual steric anomalies. An o-cyano group enhances PhCOBu triplet reactivity by stabilizing the n,π^* triplet; o-carbomethoxy deactivates PhCOBu by stabilizing the π,π^* triplet but not the n,π^* .
 IT 550-37-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and esterification of)
 RN 550-37-8 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



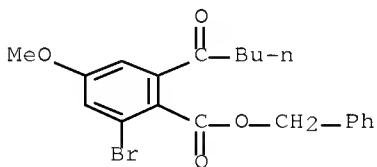
IT 64624-87-9
 RL: PRP (Properties)
 (triplet reactivity of)
 RN 64624-87-9 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 31 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1977:601488 HCAPLUS Full-text
 DOCUMENT NUMBER: 87:201488
 ORIGINAL REFERENCE NO.: 87:31903a, 31906a
 TITLE: Depsidone synthesis. X. Methoxy- and hydroxycolensoic acids
 AUTHOR(S): Djura, Peter; Sargent, Melvyn V.; Clark, Paul D.
 CORPORATE SOURCE: Dep. Org. Chem., Univ. West. Australia, Nedlands,
 Australia
 SOURCE: Australian Journal of Chemistry (1977), 30(7), 1545-51
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

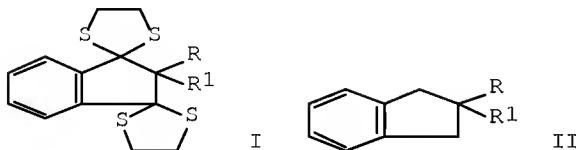


AB The synthesis of the lichen depsidones methoxycolensoic acid (I) and hydroxycolensoic acid (II) is described. An attempt to synthesize depsidones of the lobaric acid-type is also reported.
 IT 64750-36-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 64750-36-3 HCAPLUS
 CN Benzoic acid, 2-bromo-4-methoxy-6-(1-oxopentyl)-, phenylmethyl ester (CA INDEX NAME)



L28 ANSWER 32 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1977:601145 HCAPLUS Full-text
 DOCUMENT NUMBER: 87:201145
 ORIGINAL REFERENCE NO.: 87:31839a, 31842a
 TITLE: A novel synthesis of 2-substituted indans
 AUTHOR(S): Mitra, R. B.; Kulkarni, G. H.; Khanna, P. N.

CORPORATE SOURCE: Natl. Chem. Lab., Poona, India
 SOURCE: Synthesis (1977), (6), 415-17
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 87:201145
 GI



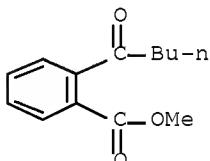
AB 1,3-Indandione bis-ketals I ($R = H, Me, Et, Pr; R1 = H, Me$) were desulfurized by Raney Ni in EtOH at reflux to give indans II. The intramol. cyclocondensation of $2-(RCHR1CO)C_6H_4CO_2Me$ in the presence of $HSCH_2CH_2SH$ gave I.

IT 64624-87-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (intramol. cyclocondensation of, and ketalization of product from)

RN 64624-87-9 HCPLUS

CN Benzoic acid, 2-(1-oxopentyl)-, methyl ester (CA INDEX NAME)



L28 ANSWER 33 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1976:577680 HCPLUS Full-text

DOCUMENT NUMBER: 85:177680

ORIGINAL REFERENCE NO.: 85:28407a, 28410a

TITLE: Synthetic studies on $(2R,4'R,8'R)$ - α -tocopherol.
 Facile syntheses of optically active, saturated, acyclic isoprenoids via stereospecific [3,3] sigmatropic rearrangements

AUTHOR(S): Chan, Ka-Kong; Cohen, Noal; De Noble, James P.; Specian, Anthony C., Jr.; Saucy, Gabriel

CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche, Inc., Nutley, NJ, USA

SOURCE: Journal of Organic Chemistry (1976), 41(22), 3497-505
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB (+)-(R)-HO₂CCH₂CHMe(CH₂)₃CHMe₂ was stereospecifically prepared from Me₂CHCH₂CHO via [3,3] sigmatropic rearrangements of (+)-(Z)- and (-)-(S)-(E)-MeCH:CHCH(OH)CH₂CHMe₂. Similarly, (+)-(R)-OCHCH₂CHMe(CH₂)₃CHMe₂ gave in very high optical purity (3S,7R)-EtO₂CCH₂CHMeCH:CHCH₂CHMe(CH₂)₃CHMe₂, which was converted into (3R,7R)-HOCH₂CH₂CHMe(CH₂)₃CHMe(CH₂)₃CHMe₂, an intermediate in the synthesis of (2R,4'R,8'R)- α -tocopherol.

IT 59983-75-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)

RN 59983-75-4 HCPLUS

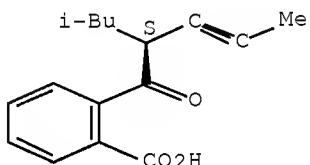
CN Benzoic acid, 2-[2-(2-methylpropyl)-1-oxo-3-pentynyl]-, (S)-, compd. with (S)- α -methylbenzenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 59983-74-3

CMF C16 H18 O3

Absolute stereochemistry.

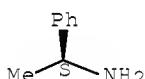


CM 2

CRN 2627-86-3

CMF C8 H11 N

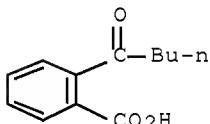
Absolute stereochemistry. Rotation (-).



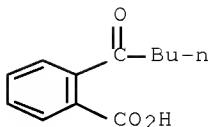
L28 ANSWER 34 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1976:58932 HCPLUS Full-text
 DOCUMENT NUMBER: 84:58932
 ORIGINAL REFERENCE NO.: 84:9675a, 9678a
 TITLE: Keto acids
 INVENTOR(S): Watanabe, Yoshihisa
 PATENT ASSIGNEE(S): Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50112319	A	19750903	JP 1974-20448	19740222
PRIORITY APPLN. INFO.:				
AB	Aliphatic or aromatic polycarboxylic acid anhydrides were treated with an iron carbonyl salt and then alkylated with an alkyl halide to give aliphatic or aromatic keto acids. Thus, 1.5 ml Fe(CO) ₅ in THF was added to Na-Hg (prepared from 0.7 g Na and 80 g Hg) in THF under Ar and Hg removed to give Na ₂ Fe(CO) ₄ . To this 1.14 g glutaric anhydride and 3.8 g BuI were added and the mixture was stirred 2 hr to give 1.32 g 5-oxononanoic acid. Similarly, succinic anhydride and BuI (MeI) gave 4-oxooctanoic acid (or 4-oxopentanoic acid); phthalic anhydride and BuI gave o-valerylbenzoic acid.			
IT	550-37-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
RN	550-37-8 HCPLUS			
CN	Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)			



L28 ANSWER 35 OF 40 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1974:504920 HCPLUS Full-text
 DOCUMENT NUMBER: 81:104920
 ORIGINAL REFERENCE NO.: 81:16583a,16586a
 TITLE: Oxidative decyanation of arylacetonitriles. Synthesis of ligusticumic acid
 AUTHOR(S): Watt, David S.
 CORPORATE SOURCE: Dep. Chem., Univ. Colorado, Boulder, CO, USA
 SOURCE: Journal of Organic Chemistry (1974), 39(18), 2799-2800
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 81:104920
 AB The oxidative decyanation of arylacetonitriles ArCH(CN)R to ketones ArCOR was effected in three steps: silylation of ArC(Li)(CN)R with Me₃CSiMe₂Cl to afford Ar-CR:C:NSi(CMe₃)Me₂, iodination of the ketenimine to afford ArC(I)(CN)R, and Ag₂O conversion of the α -iodo nitrile to ArCOR. The application of this methodology to the synthesis of ligusticumic acid is reported.
 IT 550-37-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 550-37-8 HCPLUS
 CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 36 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1964:411191 HCAPLUS Full-text

DOCUMENT NUMBER: 61:11191

ORIGINAL REFERENCE NO.: 61:1805f-h,1806e-f

TITLE: Alkylated indandiones with anticonvulsive activity

AUTHOR(S): Aebi, A.; Gyurech-Vago, E.; Hofstetter, E.; Waser, P.

CORPORATE SOURCE: CIBA Ltd., Basel, Switz.

SOURCE: Pharmaceutica Acta Helveticae (1963), 38(7-8), 407-17

CODEN: PAHEAA; ISSN: 0031-6865

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

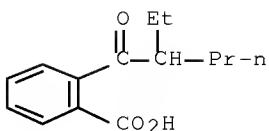
AB Alkylated indandiones with short side-chains exhibit anticonvulsive activity although they are inferior to earlier known anticonvulsives. Na (1.2 g.) in 40 ml. EtOH was heated 6 hrs. at 130-40° with 7.4 g. 2-methylindan-1,3-dione and 7 g. PrBr in a closed container to give 4.7 g. 2-methyl-2-propylindan-1,3-dione (I), m. 56-7° (EtOH). The following Ia were similarly prepared (R, R1, and m.p. or b.p. given): Me, H, (II) 86-7°; Et, H, 52-4°; Me, Me (III), 104-6°; Me, Et, 46-7°; Me, isoBu, b0.1 82-5°; Me, iso-Pr, b0.1 93-7°; Me, Bu, 41-3°; Me, Am, b0.5 120°; Me, n-C8H17, b10 153-6°; Et, Et, 15°; Et, Pr, b0.5 103-7°; Et, iso-Pr, b0.1 88-91°; Et, Bu, b0.1 105-8°; Et, isoBu, 61-3° (b0.1 104-9°); Pr, Pr, -, Bu, 71-2°; Ph, Me, 154-5°; Ph, Bu, b0.3 145-7°. Air oxiup. for 4 months at room temperature of 11 g. II gave 3.9 g. phthalic acid (IV), m. 199° (decomposition), and 0.5 g. 2-methyl-2-hydroxyindan-1,3-dione, m. 100-2° (stable indefinitely when stored under N). II (1.6 g.) in 10 ml. AcOH treated with 4 ml. 30% H2O2 overnight at room temperature and for an addnl. hr. at 40-50° gave 0.5 g. IV. II (1.6 g.) in 60 ml. N NaOH with 3 ml. 30% H2O2 0.5 hr. at 40° and overnight at room temperature gave 1.3 g. IV, which on heating to 200° gave phthalic anhydride, m. 127-9°. I (10 g.), 90 ml. 2N NaOH, and 60 ml. EtOH refluxed 18 hrs. gave 10 g. o-(2-methylvaleroyl)benzoic acid, b0.1 100°. The following o-RR1CHCOC6H4CO2H were similarly prepared (R, R1, and m.p. given): Me, Me (V), 119-21°; Me, Et, 95-7°; Me, Pr, -, Me, iso-Pr, 63-5°; Me, Bu, 45-7°; Et, Pr, -, Me, n-C8H17, 48-59°. 3-Isopropylideneephthalide, m. 93-4° (EtOH), was prepared from V by heating 2 hrs. at 200°, or by refluxing 1.9 g. V and 2 g. PC15 in 100 ml. absolute EtOH 3 hrs. III (1.75 g.) in 70 ml. AcOH hydrogenated over PtO2 at 25° and 1 atmospheric gave 0.5 g. 2,2-dimethyl-3-hydroxyindan-1-one, m. 89-90° (aqueous EtOH). III (3.5 g.) in 50 g. AcOH similarly hydrogenated gave 1.5 g. 2,2-dimethyl-1,3-dihydroxyindan, m. 159-60° (Et2O). The ultraviolet spectra of some of the compds. were reported.

IT 92864-18-1P, Benzoic acid, o-(2-ethylvaleryl)- 97024-19-6P
, Benzoic acid, o-(2-methylvaleryl)-

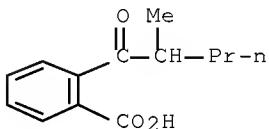
RL: PREP (Preparation)
(preparation of)

RN 92864-18-1 HCAPLUS

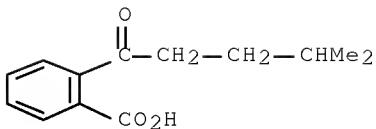
CN Benzoic acid, o-(2-ethylvaleryl)- (7CI) (CA INDEX NAME)



RN 97024-19-6 HCAPLUS
 CN Benzoic acid, o-(2-methylvaleryl)- (7CI) (CA INDEX NAME)



L28 ANSWER 37 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1954:14622 HCAPLUS Full-text
 DOCUMENT NUMBER: 48:14622
 ORIGINAL REFERENCE NO.: 48:2661f-i
 TITLE: Synthesis of alkylideneephthalides and their odor
 AUTHOR(S): Kariyone, Tatsuo; Shimizu, Shuichi
 CORPORATE SOURCE: Univ. Kyoto
 SOURCE: Yakugaku Zasshi (1953), 73, 336-8
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB RMgX (6.1 g. Mg, 50 g. Me₂CHCH₂CH₂Br, and 150 ml. dry Et₂O) treated portionwise with 20 g. powdered CdCl₂, heated 20 min., 17 g. o-C₆H₄(CO)₂O in 100 ml. Et₂O added with ice cooling, the mixture heated 1 hr., 10% H₂SO₄ added with ice cooling, the solution extracted with Et₂O, the Et₂O layer washed with 40 ml. 10% Na₂CO₃, the aqueous layer acidified with dilute H₂SO₄, and the oily layer distilled in vacuo give 15 g. o-HO₂CC₆H₄COCH₂CH₂CHMe₂ (I), b₈ 160°; I in 60 ml. 50% H₂SO₄ heated on a water bath 6-7 hrs., the product poured into cold water, and the oily product washed with 5% Na₂CO₃ and water then distilled in vacuo give o-C₆H₄.C(:R).O.CO (II) (R = CHCH₂CHMe₂), b₇ 170-2°. Other II: R = CH₂, m. 58-60°; CHMe, m. 64°; CMe₂, m. 96°; CHEt, b₁₂ 170°; CHCHMe₂, m. 97°; CHPr, b₆ 134°; CHCH:CH₂, b₆ 125-30°; CHPh (III), m. 96° (no aroma); CHC₆H₄Me-p (IV), m. 152°. 3-Butylidenetetrahydronaphthalide (V), b₇ 140-2°. The aroma of the II increases with an increasing number of C atoms in R; II with R = Pr or Bu are most similar to Ligusticum acutilobum (VI); III and IV have an unpleasant odor, although the reduction of the C₆H₆ nucleus in the phthalide resulted in an aroma similar to that of VI.
 IT 860698-74-4P, Benzoic acid, o-(4-methylvaleryl)-
 RL: PREP (Preparation)
 (preparation of)
 RN 860698-74-4 HCAPLUS
 CN Benzoic acid, 2-(4-methyl-1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 38 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1941:30348 HCAPLUS Full-text

DOCUMENT NUMBER: 35:30348

ORIGINAL REFERENCE NO.: 35:4764c-g

TITLE: Synthesis of 6,8-dimethoxy-3-alkylisocoumarin. I.
Alkylidenephthalide derivatives. (Synthesis of
lobaritonide methyl ether)

AUTHOR(S): Nogami, Hisasi

SOURCE: Yakugaku Zasshi (1941), 61, 46-51(in German, 21-4)
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Treating 45 g. 3-ethylidenephthalide in 135 cc. benzene with NO₂ in the cold gave 14 g. 3-nitroethylidenephthalide (I), C₁₀H₇O₄N, m. 124°. Treating 2 g. I with 8 g. HI (d. 1.7) and 1 g. P gave 1 g. 3-methylisocoumarin (II), C₁₀H₈O₂, m. 73-4°. 3-(α -Nitropropylidene)phthalide (prepared as above), HI and P when treated as indicated above gave 3-ethylisocoumarin, m. 76-7°. Heating of 20 g. 3,5-dimethoxyphthalic anhydride, 18 g. (BuCO)₂O and 12 g. BuCO₂Na on the oil bath at 185-210° for 2 hrs. gave 4 g. 4,6-dimethoxy-3- butylideneephthalide (III), C₁₄H₁₆O₄, m. 126-7°, and the mother liquor gave 5,7-dimethoxy-3- butylideneephthalide, C₁₄H₁₆O₄, m. 99°, and 3,5-dimethoxy-2- carboxyvalerophenone, C₁₄H₁₈O₅, m. 134°. Hydrolysis of III in acetone with concentrated HCl, followed by the decarboxylation with Cu dust, gave 2,4- dimethoxyvalerophenone (IV), C₁₃H₁₈O₃, m. 38.5°. Heating 10 g. resorcinol with 14 g. BuCO₂H and 20 g. ZnCl₂ gave 9 g. 2,4-dihydroxyvalerophenone, C₁₁H₁₄O₃, m. 63°; semicarbazone, m. 175°. Methylation of the above compound with MeI gave IV. Heating 7.5 g. 3,5-dimethoxyphthalic anhydride, 4.7 g. anhydrous EtCO₂H and 3.5 g. EtCO₂Na on the oil bath at 170-80° for 1.5 hrs. gave 1.5 g. 5,7-dimethoxy-3-ethylidenephthalide, C₁₂H₁₂O₄, m. 145°; 3,5- dimethoxy-2-carboxypropiophenone, C₁₂H₁₄O₅, m. 158°. Decarboxylation of the above compound with Cu dust gave 3,5- dimethoxypropiophenone, m. 34-5°; semicarbazone, m. 130-1°. The other compds. obtained in the above reaction are 4,6-dimethoxy-3- ethylidenephthalide, C₁₂H₁₂O₄, m. 185°, and 2,4-dimethoxy-6- carboxypropiophenone, C₁₂H₁₂O₅, m. 160°. Decarboxylation of the above compound with Cu dust gave 2,4-dimethoxypropiophenone (V), m. 75°; semicarbazone, m. 205°. Methylation of 2,4-(HO)₂C₆H₃COPr with MeI gave V.

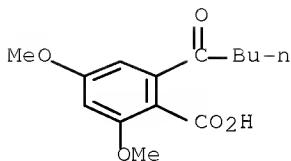
IT 855469-97-5P, Benzoic acid, 2,4-dimethoxy-6-valeryl-

RL: PREP (Preparation)

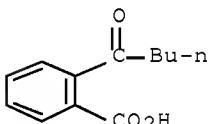
(preparation of)

RN 855469-97-5 HCAPLUS

CN Benzoic acid, 2,4-dimethoxy-6-(1-oxopentyl)- (CA INDEX NAME)



L28 ANSWER 39 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1938:24255 HCAPLUS Full-text
 DOCUMENT NUMBER: 32:24255
 ORIGINAL REFERENCE NO.: 32:3361f-g
 TITLE: Constituents of the fruits of Ligusticum acutilobum.
 III
 AUTHOR(S): Kariyone, T.; Kotani, M.
 SOURCE: Yakugaku Zasshi (1937), 57, 183-4
 From: Chem. Zentr. 1937, II, 4051
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. C. A. 31, 2583.5. Of the compds. described in the earlier paper,
 ligusticumic acid and its lactone proved to be valerophenone-o-carboxylic acid
 and butylideneephthalide, resp. (cf. Noguchi and Kawanami, preceding abstract).
 IT 550-37-8P, Benzoic acid, o-valeryl-
 RL: PREP (Preparation)
 (preparation of)
 RN 550-37-8 HCAPLUS
 CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



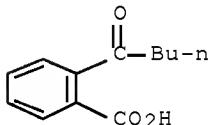
L28 ANSWER 40 OF 40 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1938:24253 HCAPLUS Full-text
 DOCUMENT NUMBER: 32:24253
 ORIGINAL REFERENCE NO.: 32:3360d-h
 TITLE: Chemical constituents of the Umbelliferae. IV.
 Constituents of Ligusticum acutilobum. 2
 AUTHOR(S): Noguchi, Takami; Kawanami, Minoru
 SOURCE: Yakugaku Zasshi (1937), 57, 196-208
 From: Chem. Zentr. 1937, II, 4050-1
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB Valerophenone-o-carboxylic acid (I), from butylideneephthalide (II) and alc.
 KOH (not pure because of lactonization), yellowish oil, b2 168-75°, gives with
 H2NCONHNH2.AcOH in alc. 1- butylphthalazonecarboxamide (III), m. 126°, which
 is converted by concentrated HCl on the water bath into 1-butylphthalazole, m.

155°, also formed from I and N₂H₄.H₂O. Butylphthalamidine, from III with Zn and HCl, m. 85-6°. Me ester of I, from I and H₂SO₄ in MeOH, yellowish, b1.5 133-4°, d₄₂₀ 1.0803, n_{D20} 1.51171. o-(Hydroxyamyl)benzoic acid, from I with H and PtO₂ in AcOH. Amide of I, from II heated with alc. NH₃, m. 134°. 1-Propylphthalazone, m. 163-4°, is obtained from N₂H₄.H₂O and butyrophenone-o-carboxylic acid (from propylenephthalide and alc. KOH), m. 88-9°. The ligusticumic acid obtained by Kariyone and Kotani (see below) from the ethereal oil of the fruits of L. acutilobum is I and ligusticumolactone is II. The crude acid also contains sedanonic acid (IV), for reduction with H and PtO₂ in AcOH gives butylphthalide and dihydrosedanonic acid (semicarbazone, m. 180°). Me ester of IV, b2.5 132-3°, d₄₂₀ 1.0326, n_{D20} 1.48088. 1-Butyl-Δ_{5,10}-tetrahydrophthalazone, from IV and N₂H₄.H₂O, m. 136°. The acid is not present as esters of dodecanol and tetradecanol, which probably are in the form of acetates, for AcOH is found in the saponification liquid. As the com. drug from the root of L. acutilobum is generally sprayed with camphor oil during storage, the greenish brown oil obtained from the roots by extraction with ether was again investigated; it contained in the acid portion palmitic, stearic, arachidic, linolic and oleic acids, in the other portion safrole, bergaptene, dodecanol, tetradecanol, butylphthalide, I, AcOH and esters of palmitic and linolic acid but no camphor.

IT 550-37-8, Benzoic acid, o-valeryl-
(and derivs.)

RN 550-37-8 HCAPLUS

CN Benzoic acid, 2-(1-oxopentyl)- (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 15:42:40 ON 15 AUG 2008)

FILE 'REGISTRY' ENTERED AT 15:42:47 ON 15 AUG 2008

L1	STR
L2	11 S L1
L3	STR L1
L4	12 S L3
L5	233 S L3 FUL
L6	STR L3
L7	105 SEARCH L6 SUB=L5 FUL
L8	STR L6
L9	17 SEARCH L8 SUB=L5 FUL

FILE 'HCAPLUS' ENTERED AT 15:51:29 ON 15 AUG 2008

L10 2 S L9

FILE 'HCAPLUS' ENTERED AT 15:52:18 ON 15 AUG 2008

FILE 'REGISTRY' ENTERED AT 15:53:14 ON 15 AUG 2008

L11 88 S L7 NOT L9

FILE 'HCAPLUS' ENTERED AT 15:53:18 ON 15 AUG 2008
 L12 25 S L11
 L13 24 S L12 NOT L10
 E SALMON R/AU
 E SALMON ROGER/AU
 L14 219 S E3 OR SALMON ROGER ?/AU OR SALMON R/AU OR SALMON R ?/AU
 E CROWLEY P/AU
 L15 150 S E3 OR E8 OR E10 OR E12 OR E14-E16
 L16 19 S L14 AND L15

FILE 'REGISTRY' ENTERED AT 15:58:54 ON 15 AUG 2008
 L17 128 S L5 NOT (L7 OR L9)

FILE 'HCAPLUS' ENTERED AT 15:59:07 ON 15 AUG 2008
 L18 28 S L17
 L19 3 S (L14 OR L15) AND L18
 L20 17 S (L16 OR L19) NOT (L10 OR L13)

FILE 'REGISTRY' ENTERED AT 16:17:56 ON 15 AUG 2008
 L21 STR
 L22 2 S L21
 L23 STR L21
 L24 6 S L23
 L25 128 S L23 FUL
 SAVE TEMP L25 RICC826FUL/A
 L26 STR L21
 L27 38 SEARCH L26 SUB=L25 FUL

FILE 'HCAPLUS' ENTERED AT 16:19:57 ON 15 AUG 2008
 L28 40 S L27

FILE 'HCAPLUS' ENTERED AT 16:20:31 ON 15 AUG 2008

=> fil reg;s 125 not 127
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 DICTIONARY FILE UPDATES: 14 AUG 2008 HIGHEST RN 1041071-62-8

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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 on property searching in REGISTRY, refer to:

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L29 90 L25 NOT L27

=> fil hcaplu;s 129
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FILE COVERS 1907 - 15 Aug 2008 VOL 149 ISS 8
FILE LAST UPDATED: 14 Aug 2008 (20080814/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

L30 48 L29

=> s 130 not 128
L31 43 L30 NOT L28

=> d scan

L31 43 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 35-6 (Synthetic High Polymers)
Section cross-reference(s): 22
TI Esterolytic activity of poly(1-methyl-4- and -5-vinylimidazole) in water
ST polyvinylimidazole esterolysis catalyst; carboxyphenyl alkanoate
esterolysis kinetics; enzyme analog esterolysis kinetics
IT Kinetics of hydrolysis
(of esters, in presence of poly(methylvinylimidazole))
IT Hydrolysis catalysts
(poly(methylvinylimidazole), for esters)
IT 56662-93-2 56662-95-4
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for hydrolysis of carboxyphenylalkanoate)
IT 2345-34-8 16358-93-3 56670-30-5 56670-31-6 56670-32-7
56670-33-8
RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrolysis of, in presence of poly(methylvinylimidazole), kinetics of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l31 and pd=<october 12, 2006
 27433844 PD=<OCTOBER 12, 2006
 (PD=<20061012)
 L32 41 L31 AND PD=<OCTOBER 12, 2006

=> d scan

L32 41 ANSWERS HCPLUS COPYRIGHT 2008 ACS on STN
 CC 10-1 (Microbial Biochemistry)
 Section cross-reference(s): 25
 TI Structures and antimicrobial activity of peniophorin A and B, two
 polyacetylenic antibiotics from Peniophora affinis Burt
 ST antibiotic peniophorin Peniophora
 IT Peniophora affinis
 (antibiotics peniophorins A and B from)
 IT Molecular structure, natural product
 (of peniophorin A)
 IT Nomenclature, new natural products
 (peniophorin A)
 IT Nomenclature, new natural products
 (peniophorin B)
 IT Fungicides and Fungistats
 (peniophorins A and B)
 IT Antibiotics
 (polyacetylenic, from Peniophora affinis, peniophorins A and B)
 IT 75217-61-7 75217-62-8
 RL: BIOL (Biological study)
 (antibiotic, from Peniophora affinis)
 IT 75235-25-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):.

L32 41 ANSWERS HCPLUS COPYRIGHT 2008 ACS on STN
 CC 10 (Organic Chemistry)
 TI Fulvic acid: its structure and relationship to citromycetin and fusarubin
 IT Fulvic acid
 (structure of, and its relation to citromycetin and fusarubin)
 IT 479-66-3
 (Derived from data in the 6th Collective Formula Index (1957-1961))
 IT 504-31-4, 2H-Pyran-2-one
 (derivs.)
 IT 109656-02-2, 1H-Naphtho[2,3-c]pyran-5,10-dione, 3,4-dihydro-3,6,9-
 trihydroxymethoxy-3-methyl-
 (fusarubin and)
 IT 4394-72-3P, 2,4,6-Octatrienoic acid, 5-hydroxy-3,7-dimethyl-,
 δ-lactone 95730-85-1P, 1H,10H-Pyrano[4,3-b][1]benzopyran-9-
 carboxylic acid, 7,8-dihydroxy-3-methyl-10-oxo- 95730-85-1P,
 1H,10H-Pyrano[4,3-b][1]benzopyran-9-carboxylic acid, 7,8-dihydroxy-3-
 methyl-10-oxo-, anhydrofulvic acid 109100-85-8P, Benzoic acid,
 2,3,5-trihydroxy-6-[2-(hydroxymethyl)-3,5-dioxohexanoyl]-
 RL: PREP (Preparation)
 (preparation of)

IT 478-60-4, Citromycetin 1702-77-8, Fusarubin
(structure of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):..

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 1-3 (Pharmacology)
Section cross-reference(s): 7
TI Receptor mapping by comparative molecular field analysis of phospholipase A2 inhibitors
ST phospholipase A2 inhibitor structure based design
IT Inflammation inhibitors
(design; receptor mapping by comparative mol. field anal. of phospholipase A2 inhibitors in relation to drug design)
IT Molecular structure-biological activity relationship
(receptor mapping by comparative mol. field anal. of phospholipase A2 inhibitors in relation to drug design)
IT 9001-84-7, Phospholipase A2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(receptor mapping by comparative mol. field anal. of phospholipase A2 inhibitors in relation to drug design)
IT 167775-07-7 167775-08-8 167775-09-9 167775-10-2
167775-11-3 167775-12-4 167775-13-5 167775-14-6 167775-15-7
167775-16-8 167775-17-9 167775-18-0 167775-19-1 167775-20-4
167775-21-5 167775-22-6 167775-23-7 167775-24-8 167775-25-9
167775-26-0 167775-27-1 167775-28-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(receptor mapping by comparative mol. field anal. of phospholipase A2 inhibitors in relation to drug design)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):..

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
CC 35 (Noncondensed Aromatic Compounds)
TI Polyacetylene compounds. CIX. Synthesis of naturally occurring, aromatic substituted acetylene compounds
IT Antispasmodics
(phenoxyalkyl amines as)
IT 1,3-Isochromandione, 3-(2-butynyl)-
2-Hexene-4,6-diyn-1-ol, 7-(m-hydroxyphenyl)-, diacetate
RL: PREP (Preparation)
IT 7387-96-4 10429-31-9 10429-32-0 13072-40-7 95159-95-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
IT 84-72-0P, Phthalic acid, ethyl ester, ester with Et glycolate 84-72-0P,
Glycolic acid, ethyl ester, ester with Et phthalate 3570-28-3P,
Isocoumarin, 3-(2-butynyl)- 4368-08-5P, o-Anisic acid,
6-(2,4-hexadiynyl)-, methyl ester 7347-83-3P, Benzophenone,
2-[2-(dimethylamino)propoxy]-, hydrochloride 7347-84-4P, Benzophenone,
2-[2-(diethylamino)propoxy]-, hydrochloride 7347-85-5P, Ammonium,
[2-(o-benzoylphenoxy)-1-methylethyl]diethylmethyl, iodide 7347-86-6P,
Piperidinium, 1-[2-(2-benzoylphenoxy)-1-methylethyl]-1-methyl-, iodide
7347-87-7P, Ammonium, diethylmethyl[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl], iodide 7347-88-8P, Ammonium, tert-butyldimethyl[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl], iodide 7347-89-9P,
Pyrrolidinium, 1-methyl-1-[1-methyl-2-[2-(phenylmethyl)phenoxy]ethyl]-,

iodide 7347-90-2P, Piperidinium, 1-ethyl-1-[1-methyl-2-[2-(phenylmethyl)phenoxy]ethyl]-, iodide 7347-91-3P, Triethylamine, 1-methyl-2-[(α -phenyl-o-tolyl)oxy]-, hydrochloride 7347-92-4P, Ammonium, trimethyl[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl], p-toluenesulfonate 7350-01-8P, Piperidinium, 1-methyl-1-[1-methyl-2-[2-(phenylmethyl)phenoxy]ethyl]-, salt with 4-methylbenzenesulfonic acid (1:1) 7387-95-3P, Ammonium, [3-[(α -hydroxy- α , α -diphenyl-o-tolyl)oxy]propyl]trimethyl, p-toluenesulfonate 7387-97-5P, Piperidinium, 1-[1-methyl-2-[2-(phenylmethyl)phenoxy]ethyl]-1-propyl-, sulfate (1:1) 10398-89-7P, 3-Isochromancarboxylic acid, 3-(2-butynyl)-1,4-dioxo-, ethyl ester 10398-89-7P, Benzoic acid, o-(2-carboxy-2-hydroxy-4-hexynoyl)-, δ -lactonet, Et ester 10401-06-6P, Anisole, 2-bromo-3-(2,4-hexadiynyl)- 10401-07-7P, 2,4-Hexadiynophenone, 2'-bromo-3'-methoxy- 10401-08-8P, 1,3-Dioxolane, 2-(2-bromo-3-methoxyphenyl)-2-(1,3-pentadiynyl)- 10401-09-9P, Cinnamic acid, m-hydroxy-, ethyl ester, benzoate 10401-10-2P, Propiolic acid, (m-hydroxyphenyl)- 10401-11-3P, Phenol, m-ethynyl- 10401-14-6P, Benzoic acid, o-(carboxyglycoloyl)-, δ -lactonet, Et ester 10401-14-6P, 3-Isochromancarboxylic acid, 1,4-dioxo-, ethyl ester 10401-15-7P, Benzoic acid, o-(2-hydroxy-4-hexynoyl)-, δ -lactone 10401-16-8P, 2,4-Hexadiyn-1-ol, 1-(2-bromo-3-methoxyphenyl)- 10401-17-9P, m-Anisaldehyde, 2-bromo-, (2,4-dinitrophenyl)hydrazone 10401-18-0P, m-Anisaldehyde, 2-bromo- 10401-19-1P, Anisole, 2-bromo-3-(dichloromethyl)- 10401-21-5P, o-Anisic acid, 6-(2,4-hexadiynoyl)-, methyl ester 10401-25-9P, Benzophenone, 2-[2-(dipropylamino)propoxy]-, hydriodide 10401-26-0P, Benzophenone, 2-[2-(dibutylamino)propoxy]-, hydriodide 10429-12-6P, Benzydrol, 2-(3-piperidinopropoxy)-, hydrobromide 10429-13-7P, Methanol, [o-[3-(dimethylamino)propoxy]phenyl]diphenyl-, hydrochloride 10429-14-8P, Methanol, [o-[3-(diethylamino)propoxy]phenyl]diphenyl-, hydrobromide 10429-15-9P, Ammonium, dibutyl[3-[(α -hydroxy- α -phenyl-o-tolyl)oxy]propyl]methyl, iodide 10429-16-0P, Piperidinium, 1-[3-[(α -hydroxy- α -phenyl-o-tolyl)oxy]propyl]-1-methyl-, iodide 10429-25-1P, Benzophenone, 2-[3-(dimethylamino)propoxy]-, hydrobromide 10429-26-2P, Benzophenone, 2-[3-(diethylamino)propoxy]-, phosphate 10429-27-3P, Benzophenone, 2-[3-(dipropylamino)propoxy]-, hydriodide 10429-28-4P, Benzophenone, 2-[3-(dibutylamino)propoxy]-, hydrobromide 10429-30-8P, Benzaldehyde, o-[3-(dimethylamino)propoxy]- 10429-33-1P, Benzydrol, 2-[3-(dipropylamino)propoxy]-, hydrochloride 10429-34-2P, Benzydrol, 2-[3-(dibutylamino)propoxy]-, hydrobromide 10429-35-3P, Propylamine, 2-[(α -phenyl-o-tolyl)oxy]-, hydrochloride 10429-37-5P, Dipropylamine, N-[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl]-, hydrochloride 10429-38-6P, Dibutylamine, N-[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl]-, hydrobromide 10429-39-7P, Diethylamine, N,1,1,1'-tetramethyl-2'-(α -phenyl-o-tolyl)oxy]-, hydrobromide 10429-40-0P, Pyrrolidine, 1-[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl]-, phosphate 10429-41-1P, Piperazine, 1-methyl-4-[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl]-, dihydrochloride 10429-42-2P, Piperidine, 1-[2-[(α -phenyl-o-tolyl)oxy]propyl]-, hydrochloride 10429-44-4P, Ethylamine, 2-[(α -phenyl-o-tolyl)oxy]- 10429-51-3P, Propylamine, N,N-diethyl-3-[(α -phenyl-o-tolyl)oxy]-, hydrochloride 10429-52-4P, Propylamine, 3-[[α -(p-chlorophenyl)-o-tolyl]oxy]-N,N-diethyl-, hydriodide 10429-55-7P, Piperazinium, 1,1-dimethyl-4-[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl]-, iodide 10429-56-8P, Dibutylamine,

N-[3-[(α -(p-chlorophenyl)-o-tolyl]oxy]propyl]-, hydrochloride 10429-57-9P, Phenethylamine, α -methyl-N-[2-[(α -phenyl-o-tolyl)oxy]ethyl]-, hydrochloride 10429-58-0P, 2-Indanamine, N-[2-[(α -phenyl-o-tolyl)oxylethyl]-, hydrochloride 10429-59-1P, Acetamide, N-2-indanyl-2-[(α -phenyl-o-tolyl)oxy]- 10429-60-4P, Acetamide, 2-(p-hydroxyphenyl)-N-[2-[(α -phenyl-o-tolyl)oxy]ethyl]- 10429-61-5P, Phenol, p-[2-[(2-[(α -phenyl-o-tolyl)oxy]ethyl]amino]ethyl]-, hydrochloride 10429-62-6P, p-Toluenesulfonamide, N-(2-hydroxyethyl)-N-(α -methylphenethyl)-, p-toluenesulfonate 10429-63-7P, p-Toluenesulfonamide, N-[2-(o-benzoylphenoxy)ethyl]-N-(α -methylphenethyl)- 10429-64-8P, Benzophenone, 2-[2-[(α -methylphenethyl)amino]ethoxy]-, hydrochloride 10446-32-9P, 2-Propanone, [p-(p-hydroxyphenoxy)phenyl]- 10571-21-8P, Benzophenone, 2-(2-piperidinopropoxy)-, hydrobromide 10602-06-9P, Benzoic acid, m-ethynyl-, methyl ester 13002-43-2P, Ammonium, [3-[(α -hydroxy- α -phenyl-o-tolyl)oxy]propyl]trimethyl, p-toluenesulfonate 13002-44-3P, Ammonium, diethyl[3-[(α -hydroxy- α -phenyl-o-tolyl)oxy]propyl]methyl, p-toluenesulfonate 13002-45-4P, Ammonium, [3-[(α -hydroxy- α -phenyl-o-tolyl)oxy]propyl]methyldipropyl, p-toluenesulfonate 13061-65-9P, m-Anisaldehyde, 2-bromo-, oxime 13072-41-8P, Morpholine, 4,4'-(2-bromo-3-methoxybenzylidene)di- 13259-72-8P, Piperidine, 1-[1-methyl-2-[(α -phenyl-o-tolyl)oxy]ethyl]-, hydrochloride 13259-73-9P, Butylamine, N,N-dimethyl-4-[(α -phenyl-o-tolyl)oxy]-, hydrochloride 13381-25-4P, Benzophenone, 2-(3-piperidinopropoxy)-, hydrobromide 93948-74-4P, Benzhydrol, 2-[3-(dimethylamino)propoxy]-, phosphate (salt) 94299-21-5P, 1,2-Pentanedione, 1-[p-(p-methoxyphenoxy)phenyl]-, 2-oxime 94876-38-7P, Benzhydrol, 2-[3-(diethylamino)propoxy]-, phosphate (salt) 879653-64-2P, Ammonium, diethyl[3-(α -hydroxy- α , α -diphenyl-o-tolyl)propyl]methyl, p-toluenesulfonate
RL: PREP (Preparation)
(preparation of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):..

L32 41 ANSWERS HCAPLUS COPYRIGHT 2008 ACS on STN
 CC 30-20 (Terpenes and Terpenoids)
 TI Efficient Construction of the Oxatricyclo[6.3.1.00,0]dodecane Core of Komaroviquinone Using a Cyclization/Cycloaddition Cascade of a Rhodium Carbenoid Intermediate
 ST oxatricyclododecane core komaroviquinone prepn cyclization cycloaddn cascade rhodium carbenoid
 IT Cyclization
 Cyclization catalysts
 Cycloaddition reaction
 (efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)
 IT 15956-28-2, Dirhodium tetraacetate
 RL: CAT (Catalyst use); USES (Uses)
 (efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)
 IT 485835-92-5P, Komaroviquinone
 RL: PNU (Preparation, unclassified); PREP (Preparation)

(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)

IT 764-59-0, 5-Hexenal 2065-66-9, Methyl triphenylphosphonium iodide
4376-18-5, Phthalic acid monomethyl ester 86549-27-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)

IT 18435-67-1P 53589-52-9P 288296-26-4P 864718-96-7P
864718-97-8P 864718-98-9P 864718-99-0P 864719-00-6P
864719-01-7P 864719-04-0P 864719-05-1P 864719-06-2P
864719-07-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)

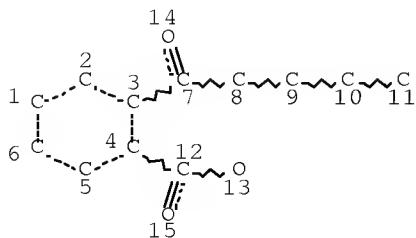
IT 864719-02-8P 864719-03-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(efficient construction of oxatricyclo[6.3.1.00,0]dodecane core of komaroviquinone using a cyclization/cycloaddn. cascade of a rhodium carbenoid intermediate)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):.

L32 41 ANSWERS HCPLUS COPYRIGHT 2008 ACS on STN
CC 35-6 (Synthetic High Polymers)
Section cross-reference(s): 22
TI Esterolytic activity of poly(1-methyl-4- and -5-vinylimidazole) in water
ST polyvinylimidazole esterolysis catalyst; carboxyphenyl alkanoate esterolysis kinetics; enzyme analog esterolysis kinetics
IT Kinetics of hydrolysis
(of esters, in presence of poly(methylvinylimidazole))
IT Hydrolysis catalysts
(poly(methylvinylimidazole), for esters)
IT 56662-93-2 56662-95-4
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for hydrolysis of carboxyphenylalkanoate)
IT 2345-34-8 16358-93-3 56670-30-5 56670-31-6 56670-32-7
56670-33-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, in presence of poly(methylvinylimidazole), kinetics of)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> => d stat que 146
L23 STR



NODE ATTRIBUTES:

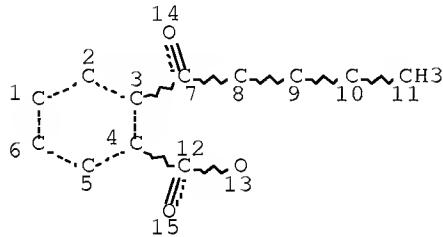
DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I
 NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L25 128 SEA FILE=REGISTRY SSS FUL L23
 L26 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I
 NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L27 38 SEA FILE=REGISTRY SUB=L25 SSS FUL L26
 L28 40 SEA FILE=HCAPLUS ABB=ON PLU=ON L27
 L29 90 SEA FILE=REGISTRY ABB=ON PLU=ON L25 NOT L27
 L30 48 SEA FILE=HCAPLUS ABB=ON PLU=ON L29
 L31 43 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 NOT L28
 L33 1609 SEA FILE=HCAPLUS ABB=ON PLU=ON LIU Q/AU OR LIU Q ?/AU OR LIU QUANZHI/AU OR LIU QUAN/AU
 L34 488 SEA FILE=HCAPLUS ABB=ON PLU=ON "YANG WENBIN"/AU OR YANG WEN/AU OR YANG WEN BIN/AU
 L35 435 SEA FILE=HCAPLUS ABB=ON PLU=ON "QIN HUA"/AU OR QIN H/AU OR QIN H ?/AU OR QIN HUA ?/AU
 L36 1893 SEA FILE=HCAPLUS ABB=ON PLU=ON ZHAO X/AU OR ZHAO X ?/AU OR ZHAO XING/AU OR ZHAO XING KAI/AU OR ZHAO XINGKAI/AU
 L37 172 SEA FILE=HCAPLUS ABB=ON PLU=ON "MA XISHENG"/AU OR MA XI/AU OR MA XI ?/AU
 L38 78 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND (L34 OR L35 OR L36 OR L37)
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 L40 85 SEA FILE=HCAPLUS ABB=ON PLU=ON L35 AND (L36 OR L37)
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 L44 117 SEA FILE=HCAPLUS ABB=ON PLU=ON (L38 OR L40) AND PD=<OCTOBER 12, 2006
 L45 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L44 AND PATENT/DT
 L46 3 SEA FILE=HCAPLUS ABB=ON PLU=ON (L39 OR L41 OR L42 OR L43 OR

L45) NOT (L28 OR L27)

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L46 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:549504 HCAPLUS Full-text
 TITLE: Pharmaceutical composition having anti-inflammatory
 and analgesic effects
 INVENTOR(S): Hu, Yingqing; Yang, Wenbin; Zhao, Xingkai; Qin, Hua
 PATENT ASSIGNEE(S): Beijing Team Academy of Pharmaceutical Science, Peop.
 Rep. China
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu
 CODEN: CNXXEV
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1682913	A	20051019	CN 2005-10051390	20050309 <--
PRIORITY APPLN. INFO.:			CN 2005-10051390	20050309

AB The title composition comprises Daemonorops draco and borneol at a weight ratio of (1-9):1, preferably (4-9):1. It has anti-inflammatory and analgesic effects and can be prepared into the forms of oral preparations such as tablet, capsule, granule, dripping pill, powder, and pill; as well as topical preparation such as plaster.

L46 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:1350280 HCAPLUS Full-text
 DOCUMENT NUMBER: 144:88042
 TITLE: Preparation of (S)-2-(1-hydroxpentyl)benzoic acid salts for treatment of cardiac ischemia, cerebral ischemia, and thrombotic diseases
 INVENTOR(S): Liu, Quanzhi; Yang, Wenbin; Qin, Hua; Zhao, Xingkai
 PATENT ASSIGNEE(S): Team Academy of Pharmaceutical Science, Peop. Rep.
 China
 SOURCE: PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005123651	A1	20051229	WO 2005-CN102	20050124 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,				

RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

CN 1594270 A 20050316 CN 2004-10048268 20040617 <--

PRIORITY APPLN. INFO.: CN 2004-10048268 A 20040617

OTHER SOURCE(S): MARPAT 144:88042

AB The title (S)-2-(1-hydroxypentyl)benzoic acid salts were prepared for treatment of cardiac ischemia, cerebral ischemia, and thrombotic diseases, and improving the circulation in heart and brain. For example, the Li, Na, K, Zn, Mg, tert-butylamine, benzylamine, and 1,2-dibenzylethylenediamine salts were prepared from (S)-2-(1-hydroxypentyl)benzoic acid and the corresponding base. The results showed that the compds. are useful as anticoagulants.

Formulations containing the title compound as an active ingredient were also described.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 3 OF 3 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:216786 HCPLUS Full-text

DOCUMENT NUMBER: 142:285151

TITLE: N, N'-dibenzyl ethylenediamine salt of 2-(alpha-hydroxypentyl) benzoic acid and its preparing process and usage

INVENTOR(S): Yang, Wenbin; Qin, Hua; Zhao, Xingkai; Ma, Xisheng

PATENT ASSIGNEE(S): Team Academy of Pharmaceutical Science, Peop. Rep. China

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005021481	A1	20050310	WO 2004-CN102	20040209 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1523003	A	20040825	CN 2003-156495	20030901 <--

PRIORITY APPLN. INFO.: CN 2003-156495 A 20030901

AB N,N'-dibenzyl ethylenediamine salt of 2-(alpha-hydroxypentyl) benzoic acid, which has significant effects in inhibiting blood platelet aggregation and improving cerebral circulation as anti-ischemic agents in the treatment of brain and heart ischemia, and cardiac or cerebral arterial embolism with good appearance, phys. state and wet stability, is provided. The preparing process of the salt, the pharmaceutical composition containing it as active component and its use in preparing medicine against brain and heart ischemia, cardiac or cerebral arterial embolism and the like are also disclosed.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

US 10/598826

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FILE 'REGISTRY' ENTERED AT 16:17:56 ON 15 AUG 2008
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L26      STR
L27      38 SEA SUB=L25 SSS FUL L26

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          D IBIB ABS HITSTR L28 1-40

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L29      90 SEA ABB=ON PLU=ON L25 NOT L27

FILE 'HCAPLUS' ENTERED AT 16:22:56 ON 15 AUG 2008
L30      48 SEA ABB=ON PLU=ON L29
L31      43 SEA ABB=ON PLU=ON L30 NOT L28
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          OR ZHAO XING KAI/AU OR ZHAO XINGKAI/AU
L37      172 SEA ABB=ON PLU=ON "MA XISHENG"/AU OR MA XI/AU OR MA XI ?/AU
L38      78 SEA ABB=ON PLU=ON L33 AND (L34 OR L35 OR L36 OR L37)
L39      4 SEA ABB=ON PLU=ON L34 AND (L35 OR L36 OR L37)
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L45      4 SEA ABB=ON PLU=ON L44 AND PATENT/DT
L46      3 SEA ABB=ON PLU=ON (L39 OR L41 OR L42 OR L43 OR L45) NOT (L28
          OR L27)
          D STAT QUE L46
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DICTIONARY FILE UPDATES: 14 AUG 2008 HIGHEST RN 1041071-62-8

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FILE COVERS 1907 - 15 Aug 2008 VOL 149 ISS 8
FILE LAST UPDATED: 14 Aug 2008 (20080814/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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